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EVALUATION OF THE BASIC GC/MS COMPUTER ANALYSIS TECHNIQUE FOR POLLUTANT ANALYSIS

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ABSTRACT

The basic gas chromatographic/mass spectrometric/computer technique for the analysis of vapor-phase organic compounds collected on a solid sorbent was evaluated. Emphasis was placed on the assessment of performance and improvement in techniques in the following areas: (1) wide bore wall coated columns for organic vapor-phase analysis; (2) gas chromatography/negative chemical ionization mass spectrometry/computer analysis of halogenated hydrocarbons in ambient air; (3) the concentration of vapor-phase organics from the atmosphere on solid sorbents (*in situ* reactions); and (4) qualitative and quantitative analysis of vapor-phase organics utilizing the improved technology.

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SECTION 1

INTRODUCTION

The need to know what chemicals may escape into the environment and at what level they may be harmful leads one to rather quickly ascertain that until compounds are identified with certainty and accurately measured, then effective controls of these chemicals is essentially impossible (1). Our society has increasingly become aware of the presence of trace amounts and sometimes far more than just trace amounts of hazardous organics which have entered the environment inadvertently or otherwise. There is scarcely any edition of a newspaper or a new magazine that does not contain a report of some new environmental mishap. The classic example is, of course, the Old Love Canal incident. Awareness has steadily increased that the ecological balance is an extremely fragile thing which can very readily be disturbed by the introduction of man-made products in a wide variety of areas. The commerical production and use of synthetic organic chemicals certainly constitutes a possible major source of insult to the ecological balance.

Synthetic organic chemical production in the United States alone has increased over the last 30 years at an annual rate of 11%. Types of direct chemical introduction are exemplified by the widespread use of pesticides, fungicides, herbicides, and insecticides, to name just a few of the organic chemicals used extensively in today's society (2).

This fact of environmental contamination coupled with Federal regulation to protect the environment from toxic chemicals has certainly placed a great burden on the analytical chemist (3). In analysis of vapor- phase organics in the atmosphere, the analyst is called upon to both identify and measure organic substances. A tremendous range of atmospheric conditions, i.e. rural to urban, and pollution sources, mobile to industrial (anthropogenic/non-anthropogenic) is encountered. Indeed, as a result there has been a heavy burden placed upon the separation sciences and instrumental development for the analysis of vapor-phase organics.

During the past several years research has been conducted on the development of a method for the collection and analysis of vapor-phase organics including carcinogenic and mutagenic substances. The developed techniques were to achieve ppt detection limits. During the development of these techniques, a number of facets have required attention for successful completion of this concept (4). A concise presentation of the overall components envisioned to encompass the analysis of organic vapors in ambient air using high resolution gas chromatography/mass spectrometry/computer has been discussed (4). This research program begins to evaluate the various components which have been assembled as a complete analytical system for organic analysis.

The objectives of this program are to improve on techniques and/or devices within this concept, and to provide the best technology available for complete characterization and quantification of vapor-phase organics in the atmosphere. This report discusses several of these areas: (1) improvements in the preparation of high resolution columns for the analysis of non-polar, semi-polar and polar organic vapor-phase constituents; (2) the increased sensitivity and specificity offered by gas chromatography negative chemical ionization mass spectrometry; (3) potential *in situ* reactions which may occur on sorbents during the collection of vapor-phase organics; and (4) the application of the improved technology to the qualitative and quantitative analysis of vapor-phase organics in ambient air from several geographical areas within the Continental U.S.

SECTION 2

CONCLUSIONS

Studies were conducted on the preparation and evaluation of wide-bore wall-coated open tubular (WCOT) columns for organic vapor-phase analysis. The previous problems associated with the use of capillary columns such as adsorption were substantially reduced with WCOTs prepared by the silanized and barium carbonate treatment methods described in this report. Columns of choice which provided a large linear dynamic range for qualitative and quantitative analysis of vapor-phase organics were 1.0 μ stationary film thick wide-bore WCOT. Columns were 0.5 mm i.d. x 75 m in length coated with SE-30 stationary phase. In conjunction with the use of capillaries for analysis of vapor phase organics, a series of performance criteria were developed which insure their chromatographic quality. The criteria were: (a) percent peak asymmetry factor (PAF) to measure the extent of overloading [capacity] and adsorption of the column; (b) effective Height Equivalent to a Theoretical plate (HETP); (c) separation number [SN]; (d) resolution; and (e) acidity and basicity. The performance mixture consists of ethylbenzene, p-xylene, octane, decane, 1-octanol, nonanone, acetophenone, 2,6-dimethylphenol and 2,6-dimethylaniline. The performance mixture was used daily to assess the capillary column's performance and develop historical data on its performance as well as to insure that the capillary continues to meet specified performance criteria for vapor-phase organic analysis.

Gas chromatography negative ion chemical ionization/mass spectrometry/computer (NICI) analysis of organic vapor phase compounds was demonstrated to be a useful method. The utility of this technique was exemplified with the determination of halogen-containing compounds in complex atmospheric samples. The technique is useful for rapid screening of samples for the presence of chlorinated, brominated and iodine-containing compounds.

Studies were conducted on in situ reactions which potentially occur as the result of the presence of criteria pollutants (ozone, NO, NO_2, NO_x), molecular halogens and olefins simultaneously occurring in the atmospheres samples. Although ozonization and halogenation of olefinic compounds were detected when atmospheres containing reactive inorganic gases and molecular halogens were collected on sorbent cartridges, the problems associated with these reactions were considerably reduced below the detection limit when the particulate filter was impregnated with sodium thiosulfate. Ozonization of olefinic compounds was detected as well as chlorination and bromination of olefins. However, difficulties exist in discerning between reactions associated with the collection device and those which are a result of a very rapid atmospheric reaction. The primary in situ reaction products that were detected when molecular chlorine was added to ambient air were chlorinated cyclohexanes derived from endogeneous cyclohexene. Also bromoform was a principal reaction product when bromine was added to the ambient air. The use of deuterated compounds in studying *in situ* reactions facilitates the differentiation between endogenous, halogenated hydrocarbons and those which are formed as a result of an *in situ* reaction when GC/MS is employed. The use of deuterated compounds is recommended when sampling reactive atmospheres containing molecular halogens. In all of the *in situ* reaction studies, ozone appeared to play a role in facilitating these reactions while in its absence they were considerably reduced.

Quantification of selected organic compounds in ambient air requires that the gas chromatographic/mass spectrometric/computer system be standardized in order to obtain reproducible and accurate data. Research was conducted to achieve reproducible and quantitative data from a mass spectrometer by incorporating a number of criteria that were delineated to serve as guidelines to achieve this objective. Perfluorotoluene was used as a standard compound to represent the m/z range of interest in the analysis and to insure that the calibration of the mass spectrometer was within specified tolerances (mass intensities) for an optimum standard spectrum. A relationship between the percent standard deviation (coefficient of variation) of the relative molar response ratios as a function of the relative retention order for selected organics was found and the highest degree of quantitative precision was obtained for the elution of internal standards near the compounds of interest. The constancy of relative molar response ratios over the dynamic mass (quantity) range of analysis was studied and found to be linear for the WCOT capillaries which were developed and evaluated under this program.

Several levels of compound identification have been delineated which defines the degree of certainty of the identify of an organic compound. The five levels of identification were: (1) computer identification [lowest level of certainty]; (2) manual interpretation; (3) manual interpretation plus retention times/boiling point of compound; (4) manual interpretation plus retention times of authentic compound; and (5) level (4) plus independent confirmation techniques.

SECTION 3

RECOMMENDATIONS

During the course of this research program, a number of areas have come to light which require further attention. Four major phases of research should be expanded and pursued:

(1) Further evaluation of capillary columns should be conducted for the analysis of hazardous [mutagenic, carcinogenic, toxic] substances collected from the ambient air. These evaluations should include the examination of the flexible fused silica columns coated with non-polar, semi-polar and polar phases. Also, narrow bore *vs*. wide-bore capillaries and thin film *vs*. thick films should be examined according to the performance criteria specified in this report. Research should be conducted on the selection of an adequate polar phase for the analysis of polar vapor-phase organics in ambient air.

(2) Research effort should be devoted to examining the optimum operating parameters for negative and positive chemical ionization of vapor phase organics. Research into a variety of reagent gases available for use in chemical ionization should be conducted to ascertain the possibility of developing operating parameters which are selective for chemical classes as well as enhanced sensitivity. Because negative ion chemical ionization is a relatively new tool, this area of research appears to be virgin and requires considerable study to fully utilize the selectivity and high sensitivity of this method.

(3) Additional studies are recommended on potential *in situ* reactions associated with the Tenax GC collection device. Particular emphasis should be placed on the potential artifacts which may occur under field sampling conditions and, if any problems exist, to delineate procedures which might deplete or scavenge the reactive gases prior to the collection of the organic vapor-phase fraction.

and (4) The use of deuterated internal standards should be developed for the quantitative collection and analysis of vapor-phase organics. Techniques for the sparging of ambient air with deuterated compounds during the sampling period should be developed in order to provide a means for the assessment of the collection efficiency and recovery of vapor-phase organics as well as to uncover any potential in situ reactions which might have occurred during ambient air sampling.

SECTION 4

PROGRAM OBJECTIVES

The overall broad term objective was to evaluate methodology encompassing the use of a solid sorbent collection device for the collection of vapor-phase organics in combination with gas chromatography/mass spectrometry/computer for their analysis. The specific aims of this program were to evaluate this methodology while applying it to 10 different sites within the Continental U.S. The limitations and the overall analysis capability were documented with research improvements to be implemented to correct any uncovered deficiencies. This program was divided into four general objectives:

(1) To collect and analyze samples from one site for a minimum of 4-5 days to obtain qualitative and/or quantitative data concerning selected vapor-phase organics occurring in ambient air. These data were to be reduced and presented in reports to the Project Officer and any improvements in the analytical methodology necessary to achieve the desired results were to be documented prior to the next site visit. Additional sites were to be visited in sequence with essentially the same format: namely, effecting what improvements were necessary to maximize analysis capability. During field evaluation of techniques qualitative and quantitative analysis of ambient air samples for selected constituents was also to be performed.

(2) To summarize the overall analysis capability highlighting and recommending innovations or revisions in the methodology made as a result of the test studies conducted while applying the capability at the sites visited.

(3) To provide a listing of suspected toxic pollutants which were identified in ambient air samples. Particular emphasis was to be placed upon known or suspected carcinogens and profiling these pollutants endemic to each site as they were studied.

and (4) To transfer the latest technological improvements developed under this research program to the on-going EPA in-house research effort. To furnish any necessary hardware and/or technology and to demonstrate the operation of the methodology for the EPA's in-house function.

As part of this objective, full documentation was to be provided for the new technical developments or modifications made as a result of the evaluation of the basic GC/MS/computer analysis system.

SECTION 5

PREPARATION OF WIDE BORE WCOT COLUMNS FOR ORGANIC VAPOR-PHASE ANALYSIS

GENERAL OBJECTIVES

One of the objectives of this program has been to improve on the glass capillary technology which is used in the basic GC/MS method for analysis of vapor-phase organics in ambient air. Problems associated with the columns previously employed such as SE-30 or OV-101 coated SCOT columns have been the extraordinary adsorption of polar organic components which are collected and thermally desorbed from the Tenax GC sampling cartridge. In general the SCOT columns were adequate for the analysis of non-polar and semi-polar materials, e.g., alkanes, alkyl aromatics, halogenated hydrocarbons and oxygenated compounds such as aldehydes and ketones. However, with the more polar substances these columns exhibited a high degree of adsorption during chromatography of low levels (ppt) of organics. This problem is unacceptable for two reasons. First, it precludes the chromatography of acidic compounds such as phenols and bases. Secondly, when adsorption of organics on the capillary column becomes significant, then the use of relative molar response factors becomes invalid. This is due to the non-linearity of response when chromatographing low quantities of organics. For accurate usage of relative molar response factors, linearity of response over the dynamic range of interest and the extrapolation of the response curves through an intercept of zero is necessary.

In addition to the problem of adsorption on SCOT capillaries, the reproducible preparation of the SCOT capillary with silanized fumed silicon dioxide as the support has been difficult. The quality of commercially available material has varied from batch to batch. The quality control steps employed in our laboratory for the preparation of SCOT capillaries requires testing the silanized fumed silicon dioxide with a solution of methyl red to ascertain whether it is neutral. This simple test has revealed batch to batch variations.

For these reasons, an investigation into the preparation of wide bore WCOT columns for the analysis of organic vapor-phase compounds was instituted. Furthermore, while retaining capacity, the resolution of these columns is superior to the SCOT. This section discusses the characteristics of WCOT columns, their preparation, performance, and their application to the analysis of vapor-phase organics in the ambient air (Section 8).

INTRODUCTION TO WCOTS

There are several arguments for preparing capillaries in a research laboratory. Among these arguments are that they offer an opportunity for investigators to acquire a better understanding of this basic tool. It also allows for more useful applications of the technique to a variety of problems which otherwise would be limited to what is commercially available. Finally one of the major advantages is that the full usage of this technique is possible since the researcher may tailor-make the capillary to fit a specific analytical problem.

A discussion of glass capillary technology is presented which has been synthesized from a number of literature sources with the major contributions from K. Grob's laboratory (7).

Characteristics of Glass/Quartz

Among the merits of glass/quartz *vs*. metal as a support or container for the stationary phase are that it is: (1) transparent; (2) readily available; and (3) offers a variety of approaches for the modification of the surface for tailor-making columns. However, it is not without its problems since quartz is ill-defined and can be considered as a "quasi-liquid" material, *i.e.*, there is always some internal diffusion of metal ions. It has been demonstrated that the leaching of heavy metal ions from the surface of glass (soft and pyrex) is only a temporary solution since after a period of time and particularly at elevated temperatures, the heavy metal ions migrate from the internal matrix to the surface (5). However, it is still necessary to remove metal ions from the surface since they can be involved in catalytic decomposition of organics during chromatography. Thus, all glass materials must be pretreated by a method which leaches the calcium, magnesium, iron, boron and lead that occur with different types of glasses.

A variety of glass types are available. In fact, this is one of the major disadvantages with the use of glass as a container. In general pyrex glass can be considered to be acidic, brittle and more compact in structure than soft glass which is generally basic, has a more open structure and is relatively stable mechanically. Because of the open structure of the soft glass, the tendency for metal ions to migrate in the matrix is greater than with pyrex. Fused silica has the lowest quantity of metal ions (6).

Requirement of Column Preparation

There are three general requirements in the preparation of wall coated open tubular columns: (1) achieving wettability; (2) good deactivation; and (3) high thermal stability. During the preparation of coated glass capillary columns, it is important that the film of stationary phase is homogeneous throughout the open tubular column since this gives the highest separation efficiency. When drops or pools of stationary phase form a reduced efficiency is observed. The glass surface must be entirely deactivated, *i.e.*, there are no active sites which can participate in catalysis or adsorption. Deactivation includes removal of metal ions and chemically shielding polar groups (*e.g.*, silanol). When a homogeneous film and good deactivation are achieved, then the column will exhibit excellent thermal stability and high efficiencies.

There are two principal forms of wetting (7). The first involves intermolecular forces between the stationary phase and the glass wall. This constitutes "chemical" wettability. It may be achieved through hydrogen bonding, π-π interactions or Van der Waals forces. The use of the σ charge transfer such as observed with nitrile bonding has often failed to provide chemical wettability. A second type of wettability is "topographic" or "geometric". Essentially this constitutes the roughening of the surface to produce a lower contact angle between the stationary phase and the glass surface. The topographic wetting produces a "quasi-film"; a reduced efficiency is observed. In practice a combination of the two forms to achieve wetting may be necessary; however, this is dictated by the interaction between the phase and the glass capillary wall. For example, with an apolar phase a smooth inactive surface is sufficient. With a moderately polar stationary phase, a roughened surface that has been inactivated is generally the best compromise. Finally, with polar stationary phases, a rough and active surface allows for the best wetting or most homogeneous film.

There are two generally accepted procedures for the deactivation of the glass surface. The first involves the production of a "surface bonded layer" of polar compounds with a glass wall. This is achieved by using compounds such as Carbowaxes, triethanolamines, etc. The advantages of this approach is that the deactivation is an easy step to execute and deactivation can be selective for specific compound types. The disadvantage occurs in its thermal stability where the upper limit is ∿250°C with the Carbowax 20M method. The second procedure for deactivation involves silylation. The greatest advantage of this approach is in its thermal stability which can be >350°C. The problem associated with silylation is that the surface of the silica needs to be properly prepared which is difficult and can result in reduced efficiency because of poor film stability even when using apolar phases. The principal utility of silylation is obviously to eliminate the oxide phase on the glass surface. To be successful, it is necessary to maximize the density of the silanol groups and minimize dehydration which occurs inevitably during the drawing of glass capillaries because of the high temperatures required to soften the glass. Also it is necessary to remove excess water prior to instituting the reaction. In general, the best results are obtained with hexamethyldisilazane which has been reported by Grob (7).

One of the principal approaches developed by Grob for roughening the surface of a glass wall is the "barium carbonate method". This approach is for roughening only and not deactivating the glass column. The primary purpose of a roughened surface is to increase the thermal stability of the stationary film. The extent of the roughening is controlled by the starting concentration of barium hydroxide which is converted to barium carbonate crystals via CO_2 gas. For polar phases, a saturated solution is employed while a 1:5 and 1:30 dilution is used for moderately polar and apolar stationary phases, respectively. According to Grob (7) the orientation of the barium carbonate crystals is important for the production of a highly efficient column. For example glass surfaces which have not been leached to remove ions yield barium carbonate needles standing in an erect position while a leached glass surface produces needles lying down. The barium carbonate roughened surface of a glass open tubular column can be considered as slightly basic; however,when using a highly diluted barium hydroxide solution with an extensively leached surface, it will be slightly acidic.

Other methods of roughening such as the etching of soft glasses produces sodium chloride crystals; however, these are less stable to the presence of water in the samples while not being any more active than barium carbonate crystals. The production of sodium chloride crystals is less reproducible than production of barium carbonate (7).

Coating Methods

There are three fundamental methods for coating a stationary phase on the surface of a glass capillary column. These are static, static/forced evaporation, and dynamic. The static method simply involves filling of glass capillary column with the stationary phase dissolved in an appropriate solvent at a concentration whereupon after evaporating the solvent, the stationary film is formed at an exactly predictable thickness. Upon filling the capillary, one end is sealed and then a vacuum is applied to the open end.

The forced evaporation method has been described by several investigators (7). The column after filling is sealed at one end and the open end is screwed through a heated zone which vaporizes the phase/solvent mixture. The stationary phase is "sprayed" and adheres to the surface of the glass.

The dynamic method requires pushing a plug of stationary phase/solvent mixture through the capillary using a mercury plug behind the coating solution. The film thickness produced depends upon the viscosity of the solution and the velocity used. The deposited film is subject to evaporation-condensation of the solvent as it passes through the capillary. The technique generally cannot be used with gum-type phases. The use of the mercury plug facilitates the dynamic coating method; however, some solvents such as acetone are not suitable (7).

Column Evaluation

During the evaluation of glass capillary columns, documentation of performance is required for: (1) adsorption [by the use of polar test compounds]; (2) acidity/basicity [by the use of acid and base in the test mixture]; (3) separation efficiency [by the use of a pair of homologs which do not adsorb]; and (4) film thickness [which is related to capacity and is established by the elution temperature for a reference standard component].

Adsorption characteristics can be expressed in two ways. The first may be exhibited by a process which produces tailing or broad chromatographic peaks with an incorrect area for the compound relative to the amount that was chromatographed. In the second case, adsorption may be expressed by a perfectly symmetrical chromatographic peak; however, the area is reduced with respect to that which theoretically should have been obtained for the amount chromatographed. Thus, reduced sensitivity is observed. In the first case, the adsorption may occur via a mechanism which is reversible whereas in the second it is not.

Adsorption expressed as chromatographic peak tailing may be traced to active sites in the column which may be due to hydrogen bonding, π-π interaction, or complexation with metal impurities. A test mixture which contains 1-octanol, n-nonanone, and naphthalene facilitates the differentiation of these types of adsorption. Adsorption undergoing the second mechanism generally can be attributed to acidity or basicity of the column. To detect these properties, 2,6-dimethylaniline and 2,6-dimethylphenol are often used. However, these compounds only reveal relatively strong acid/base characteristics of the capillary. To demonstrate weakly acidic and basic characteristics in a chromatographic column, 2-ethylhexanoic acid and dicyclohexylamine may be used (7).

MATERIALS AND METHODS

Drawing Capillaries

Glass capillaries were drawn from 1.22 m lengths of pyrex glass (8 mm o.d. x 4 mm i.d.) to yield an internal diameter of either 0.36 mm or 0.47 mm using a Hupe and Busch (Hewlett-Packard Corp., Avondale, PA) or Shimadzu (Seisakusho LTD, Koyoto, Japan) drawing machines. The pyrex glass tube was washed with 50 mL each of 1N HCl, water and dried with acetone prior to drawing.

Pretreatment of Capillaries

Acid Leaching--

To produce a pure silica surface by eliminating any oxide layer and to produce a maximum density of silanol groups, acid leaching was performed on the capillary. The capillary column was filled with 20% HCl by introducing the HCl solution into 10% of the total capillary length. An inert gas (N_2) was used to force the HCl solution through the capillary and the process was continued until 2% of the solution remained in the capillary. The filled end of the capillary was flame sealed and the open end connected to a vacuum source. A vacuum was created in the capillary for ~5 min and the end was flame sealed prior to disconnecting the vacuum. The capillary was then heated at 180°C for ~18 h. Upon cooling, the capillary was opened at both ends and the remaining HCl solution was slowly displaced by introducing distilled water which filled ~25% of the capillary volume. Immediately following the water plug, an equal volume of methanol was introduced.

Capillaries designated for the $BaCO_3$ method were heated for 5 h at 260-280°C under a low flow of nitrogen gas (e.g., 0.2 atm/50 m length). For capillaries to be silanized, the glass column was heated to 250°C with both open ends connected to a vacuum source (water aspirator) outside the oven. The column was heated for 18 h (for US pyrex glass).

Barium Carbonate Roughened Surface--

Solutions of $Ba(OH)_2$ (B1-saturated, B2-1:5 of saturation, and B3-1:30 of saturation each containing 4, 2 and 1 ppm of Marlazin L10, respectively) were prepared.

Into ~5 coils of the previously HCl leached and dehydrated capillaries, 0.5% HCl was drawn. The appropriate $Ba(OH)_2$ reagent (B1-B3) was drawn into 10 coils of the capillary with an air plug interposed between the HCl and $Ba(OH)_2$ solutions. An air plug was then also introduced at the rear end of the $Ba(OH)_2$ solution (inlet end of the capillary) (~20 cm long for B1 and B2 and 50 cm for B3). While protecting the column from temperature gradients, CO_2 gas was flushed into the capillary to move the solutions at a rate of 1.5 - 2 cm/sec (25-30 sec/40 cm coil). Care was instituted to prevent the interruption of the carbon dioxide flow. The exit end of the capillary was connected to a "buffer" column of a similar internal diameter and ~5-10 m in length. As soon as the rear meniscus of a $Ba(OH)_2$ solution entered into the buffer column, the CO_2 gas supply was replaced by an inert gas such as nitrogen at a pressure of 0.2 atm. After ~10 min, or when the CO_2 was flushed from the column, acetone was introduced into ~25% of the column length at a rate of 2-3 cm/sec (15-20 sec/40 cm coil) and passed through to dry it. Vacuum was applied to one end for 5 min and the column was then dried in an oven at 280°C for 30 min at 0.3-0.5 atm of N_2.

For glass capillaries treated with the B1 solution, the capillary was directly coated with polar stationary phases. For the B2 treated columns, further preparation was necessary. The glass capillary was quickly rinsed with a 1% solution of Carbowax 1000 in CH_2Cl_2 at a rate of 20 sec/coil. Both ends of the capillary were connected to a vacuum source via a tee and the vacuum applied for 5 min. Both ends of the column were then flame sealed prior to disconnecting the vacuum source. The capillary was heated to 280°C for 18 h. Upon cooling, the ends were cut and fire polished and rinsed with methylene chloride. The glass capillary column containing $BaCO_3$ from B2 treatment was then ready for coating with moderately polar phases such as OV-17 and nitrile phases.

For capillaries prepared with the B3 $Ba(OH)_2$ solution, the columns were quickly rinsed with 0.1% solution of Triton 300 in CH_2Cl_2. A vacuum was applied to one end for 5 min. With the application of a 0.2 atm pressure of inert carrier gas (N_2), the capillary was then heated to 250°C for 30 min. Upon cooling, the capillary was then rinsed with CH_2Cl_2 and dried under N_2 flow. This column was then ready for coating with apolar phases.

Deactivation by Silanization--

To produce essentially a totally non-adsorptive and non-catalytic surface with extreme heat stability in capillaries, a silanization technique was employed. Hexamethyldisilazane (Applied Science, State College, PA) was drawn into a dehydrated capillary until ~10% of the capillary length was filled with the reagent. Using a head pressure of N_2 gas, the reagent was pushed through the capillary at a rate of ~2 cm/sec. No buffer column was employed. When the reagent had passed through the capillary, the gas supply was immediately disconnected and a vacuum was applied to both ends via a tee. A vacuum was applied for ~5 min for a 20 m length (10 min for 50 m and 15 min for 75 m). Both ends of the capillary were flame sealed prior to disconnecting the vacuum. The capillary was then heated to 400°C for 12 h.

The degree of silanization is checked by breaking one of the ends of the capillary under toluene. When a few coils were filled with toluene from the vacuum, the column was switched to methanol and then to ether. When the front end of the toluene plug ceased to move, the length of the empty tubing was noted. As a general rule, 5-10% of the total length which remains empty indicates mild silanization while 20-50% of an empty column indicates heavy silanization. The second end of the capillary was opened and the liquids were forced through the capillary by applying N_2 gas to the end which contained ether. Various intensity of silanization produces powdery plugs which can impair movement. The problem can be overcome by gently warming the plugged area with a small flame. The capillary was then ready for coating with apolar phases.

Coating Techniques

Static--

The coating solution was prepared according to the desired film thickness (FT). This is given by the following relationship:

$$\mathrm{FT}\ (\mu\mathrm{M}) = 0.25\ D\ (\mathrm{mm}) \times C.$$

where D = the internal diameter,
C = the concentration of phase in parts-per-thousand (W/V)

For apolar and polar stationary phases, n-pentane and methylene chloride were the solvents used, respectively. In all cases the solutions were freshly prepared except for gum phases which were allowed to sit for ~4 hrs after mixing with the solvent.

One end of the capillary column was inserted through a silicone rubber fitting into the coating solution. The bottle containing the coating solution was connected to a source of N_2 gas at ~0.5 atm, and the capillary was filled with coating solution and flushed with an additional 25% (of column length) with coating solution. The gas pressure then was reduced to 0.1 atm and the exit end of the column was inserted into water glass. This procedure insures that small air bubbles are flushed from the column end. The inlet end of the capillary was then removed from the bottle containing the coating solution. A low pressure was applied to the inlet end to push the meniscus of the water glass to a few cm from the end. The pressure was then disconnected. The water glass bottle was tilted in such a way that the column end was located in the water glass and not contaminated with coating solution. A low vacuum was immediately applied to the inlet end to move the meniscus 1-2 cm. The exit end was removed from the water glass and immediately the excess water glass was wiped from the capillary end. The water glass and interface to the coating solution were checked for gas bubbles. In the event that there were any, the procedure was repeated by cutting the water glass plug and applying low pressure to the inlet end. This method of sealing was conducted in order to avoid the introduction of air bubbles between the water glass and the coating solution. The column was then allowed to sit for 6-8 h or overnight prior to evaporation of the solvent.

The capillary column was inserted into a water bath at room temperature with both ends ~6 cm out of the bath. The open end of the capillary was then attached to a vacuum source (water aspirator) and a low vacuum was initially applied and then a higher vacuum when the solvent meniscus had moved to the interior of the capillary. For capillaries >50 m in length the water bath was slowly heated to 40°C over a 1 h period.

Once the solvent had evaporated the closed end was opened. The vacuum was continued for a few minutes and then disconnected. The capillary was then prepared for installation.

Static/Forced Evaporation--
The coating of glass capillaries using a forced evaporation technique has been previously reported (8).

Dynamic--
Into an empty glass capillary column, a plug of coating solution was drawn (10-15 coils). Immediately following the coating solution, a 10 cm plug of mercury was also drawn. Then the column was subjected to a gas pressure head at the end containing the mercury plug and the mercury plug was pushed through the column at a rate ~1 min/turn. A buffer column was attached to the other end of the capillary in order to maintain a uniform velocity of the coating solution. During the dynamic coating process, the capillary was also protected from temperature gradients.

Preparation of Capillary Ends for Installation

Straightening of capillary ends which had been coated with stationary phase was accomplished by using oxygen or air flowing through the column during the straightening process. Prior to straightening, capillaries containing film thicknesses of 0.8-1.0 microns were washed free of phase by introducing solvent into 1-1 1/2 coils of the column using a 100 μL syringe. This step was also performed under a positive pressure. Straightening was accomplished by slowly rotating the capillary into a small microflame (1/2-1" in length), allowing gravity to pull the softened glass. The column ends were flamed to avoid problems with insertion through ferrules or septa.

Hexane was used to remove silicone oils and gums from columns which had been straightened while CH_2Cl_2 was used for Carbowaxes and other polar phases. Injection and withdrawal was repeated three times. The capillary ends were then deactivated by introducing a solution of 0.1% Carbowax 1000 in CH_2Cl_2.

RESULTS AND DISCUSSION

Performance Criteria

The glass capillary columns were evaluated according to the following criteria:

(1) percent peak asymmetry factor (PAF)

$$\%\ \text{PAF} = \frac{B}{F} \times 100$$

where B = the area of the back half of a chromatographic peak
F = area of the front half of the chromatographic peak both measured 10% above baseline

(2) effective Height Equivalent to a Theoretical Plate (HETP_{eff})

$$\text{HETP}_{eff} = \frac{L}{5.54\ (X/Y)^2}$$

where X = the corrected retention distance for sweep time of the compound,
Y = chromatographic peak width at 1/2 peak height,
L = column length (mm)

(3) separation number (SN)

$$\text{SN} = \frac{D}{W_1 + W_2} - 1$$

where D = the distance between two peaks,
W_1, W_2 = widths at 1/2 height

(4) resolution (R)

$$R = \frac{2\ \Delta W}{W_1 + W_2}$$

where ΔW = average base width,
W = peak width at base.

(5) Acidity and Basicity

$$\text{Acidity} = \frac{\text{weak base (peak area or height)}}{\text{acetophenone (peak area or height)}}$$

$$\text{Basicity} = \frac{\text{weak acid (peak area or height)}}{\text{acetophenone (peak area or height)}}$$

These criteria were used to assess the preparation of a number of glass capillary columns to delineate a systematic method for discerning the utility of glass capillary columns for ambient air pollution analysis. Performance criteria are necessary in order to provide quality control and quality assurance on the analysis of ambient air samples utilizing GC/MS/COMP with glass capillary columns. An important aspect of analysis with glass capillary columns is the continual assessment of the performance of a new column as it ages in order to discern when the column is no longer useful for this type of analysis. The criteriona of percent peak asymmetry factor has been incorporated as a quality control step in the selection and usage of capillary columns for ambient air pollution qualitative and quantitative analysis. The compounds which have been selected for assessing the performance of the columns are: 1-octanol, 5-nonanone and acetophenone. The use of these compounds provides information as to the degree of adsorption and the type of adsorption mechanisms during the interactions between solute molecules and the glass capillary wall. 1-Octanol serves as a means of determining the extent of deactivation of the glass surface and principally singles out adsorption due to hydrogen bonding. The hydrogen bonding which may occur results from incomplete deactivation of the silanol groups on a glass surface. Furthermore, the use of 5-nonanone assesses the extent of adsorption occurring from a π-π adsorption mechanism. Finally, adsorption of acetophenone incorporates the characteristics of 5-nonanone plus the aromatic π ring system of acetophenone which assist in the determination of the extent of the adsorption due to the presence of metal impurities on the glass surface.

The acidity and basicity of the capillary column are assessed by the adsorption of weak bases and acids, respectively. This performance test involves the chromatography of 2,6-dimethylaniline and 2,6-dimethylphenol and their respective peak areas (or heights) are ratioed to the peak area for acetophenone. Thus if the percent asymmetry factor is low for acetophenone (<250%), then the acidity and basicity of the column can be assessed using this relationship. In particular the capillary columns prepared by the barium carbonate procedure exhibit a slight basicity and thus the irreversible adsorption of 2,6-dimethylphenol is observed.

Finally the resolution and separation number of a column is determined in order to insure that the complex ambient air pollution mixture can be adequately resolved for the qualitative and quantitative analysis to be performed. For this purpose, the resolution between ethylbenzene and p-xylene and the separation number for octane and decane are determined.

Case Examples of Performance Evaluation of Glass Capillary Columns

Table 1 presents the results for the evaluation of a commercial glass capillary column. The resolution, separation number, percent asymmetry factor and acidity and basicity of the column are given. In general the column exhibits very low adsorption characteristics and is acceptable for the analysis of semi-polar compounds. The column exhibits slight acidity. The resolution as measured for ethylbenzene and p-xylene is ~1 while the separation number is 50. Figure 1 presents the chromatogram obtained utilizing the operating parameters for the GC/MS/COMP system given in Section 8. The performance mixture contained perfluorobenzene, perfluorotoluene, ethylbenzene, p-xylene, octane, decane, 1-octanol, 5-nonanone, acetophenone, 2,6-dimethylaniline and 2,6-dimethylphenol which were loaded onto Tenax GC sampling cartridges and then thermally desorbed using the standard conditions described in Section 8. The commercial capillary was an SE-30 wall coated open tubular with the dimensions of 0.5 mm i.d. x 27 m in length. The film thickness was 0.41 microns. Figures 2-11 present the single ion plots for the components in the performance mixture.

Table 1. EVALUATION OF A COMMERCIAL GLASS CAPILLARY[a]

Parameter	Test Compound	Value
Resolution	Ethylbenzene:p-Xylene	1.0
Separation No.	Octane:Decane	50
% Peak Asymmetry Factor	1-Octanol Nonanone Acetophenone	200% 120% 150%
Acidity	2,6-Dimethylaniline:Acetophenone	0.7
Basicity	2,6-Dimethylphenol:Acetophenone	0.9

[a] SE-30 WCOT, 0.5 mm i.d. x 27 m, 0.41 μ film thickness.

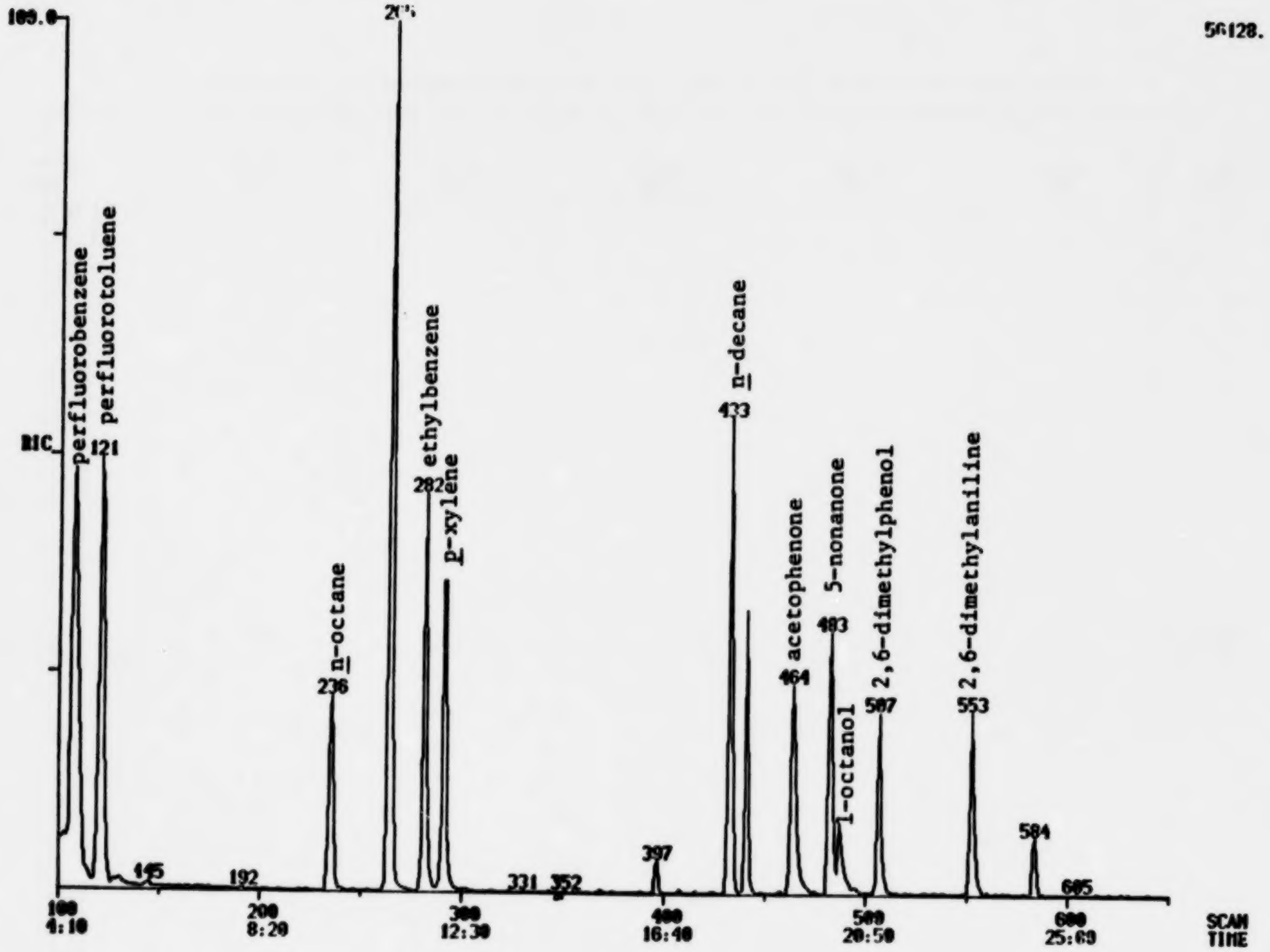


Figure 1. GC/MS/COMP profile of performance mixture for capillary column evaluation (SE-30 WCOT, 0.5 mm i.d. x 27 m, 0.41 μ film thickness; 30-250°C @ 4°C/min).

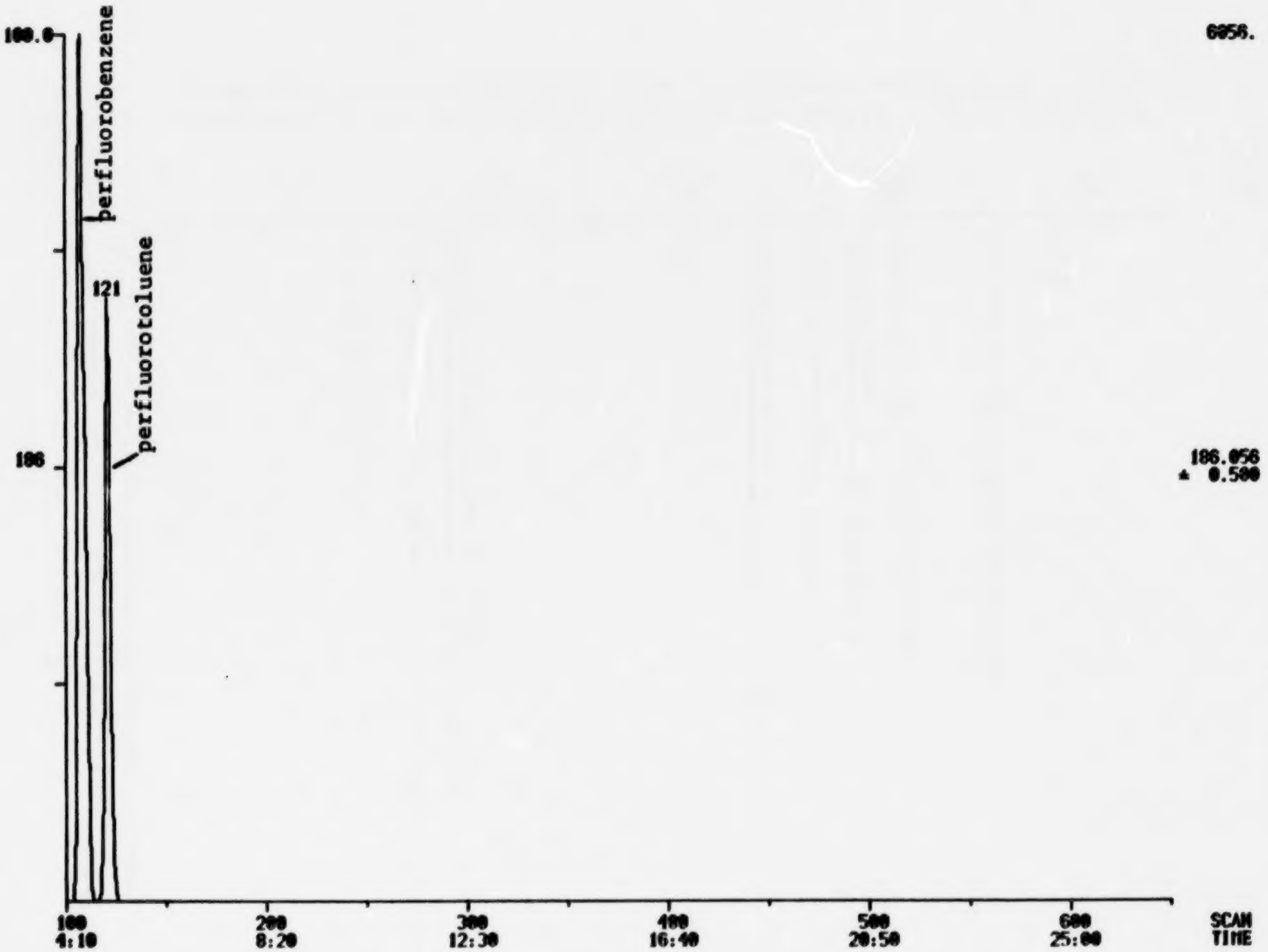


Figure 2. Extracted ion current profile of m/z 186 for perfluorobenzene and perfluorotoluene in performance mixture (see Fig. 1 for operating conditions).

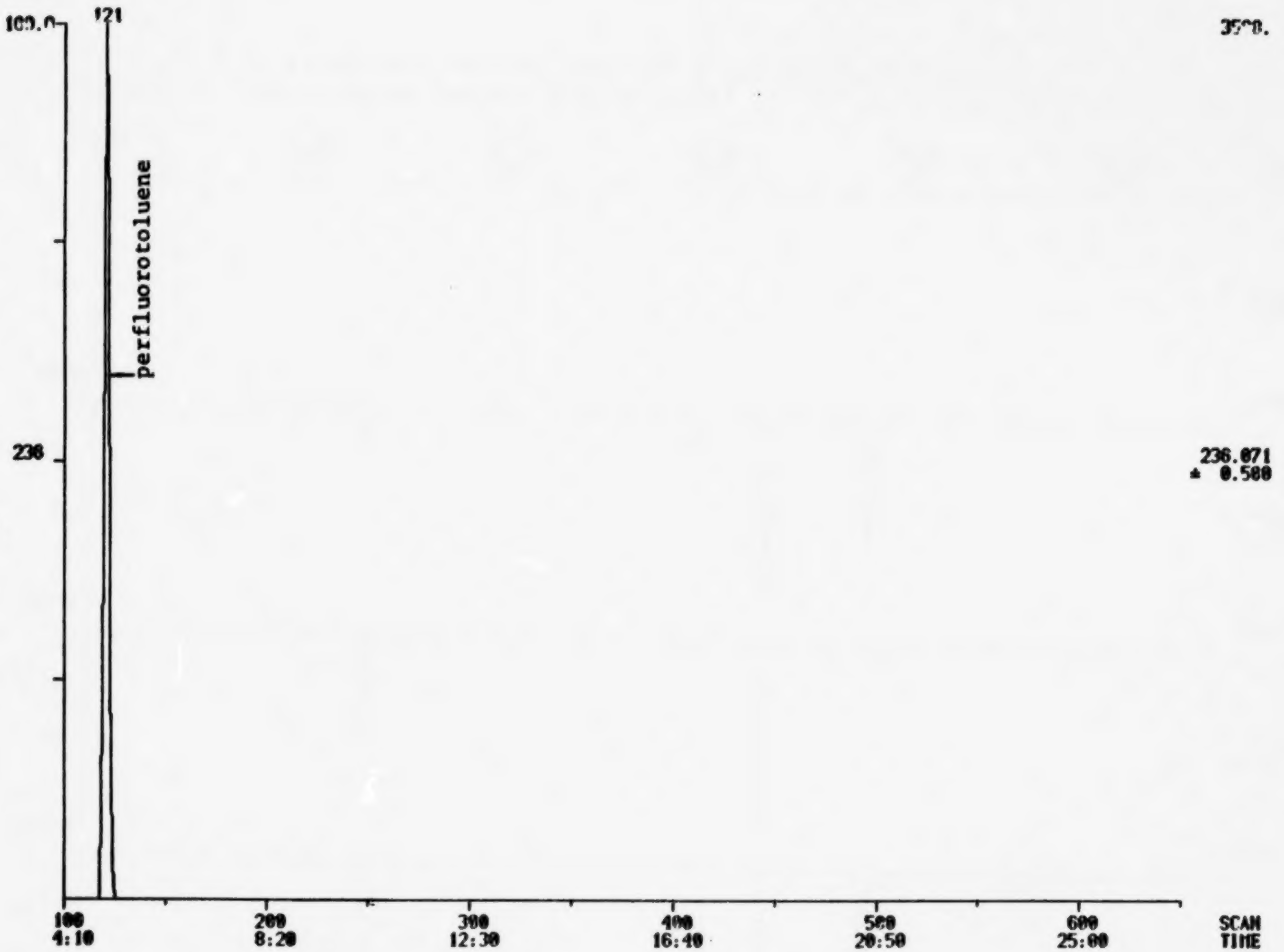


Figure 3. Extracted ion current profile of m/z 236 for perfluorotoluene in performance mixture (see Fig. 1 for operating conditions).

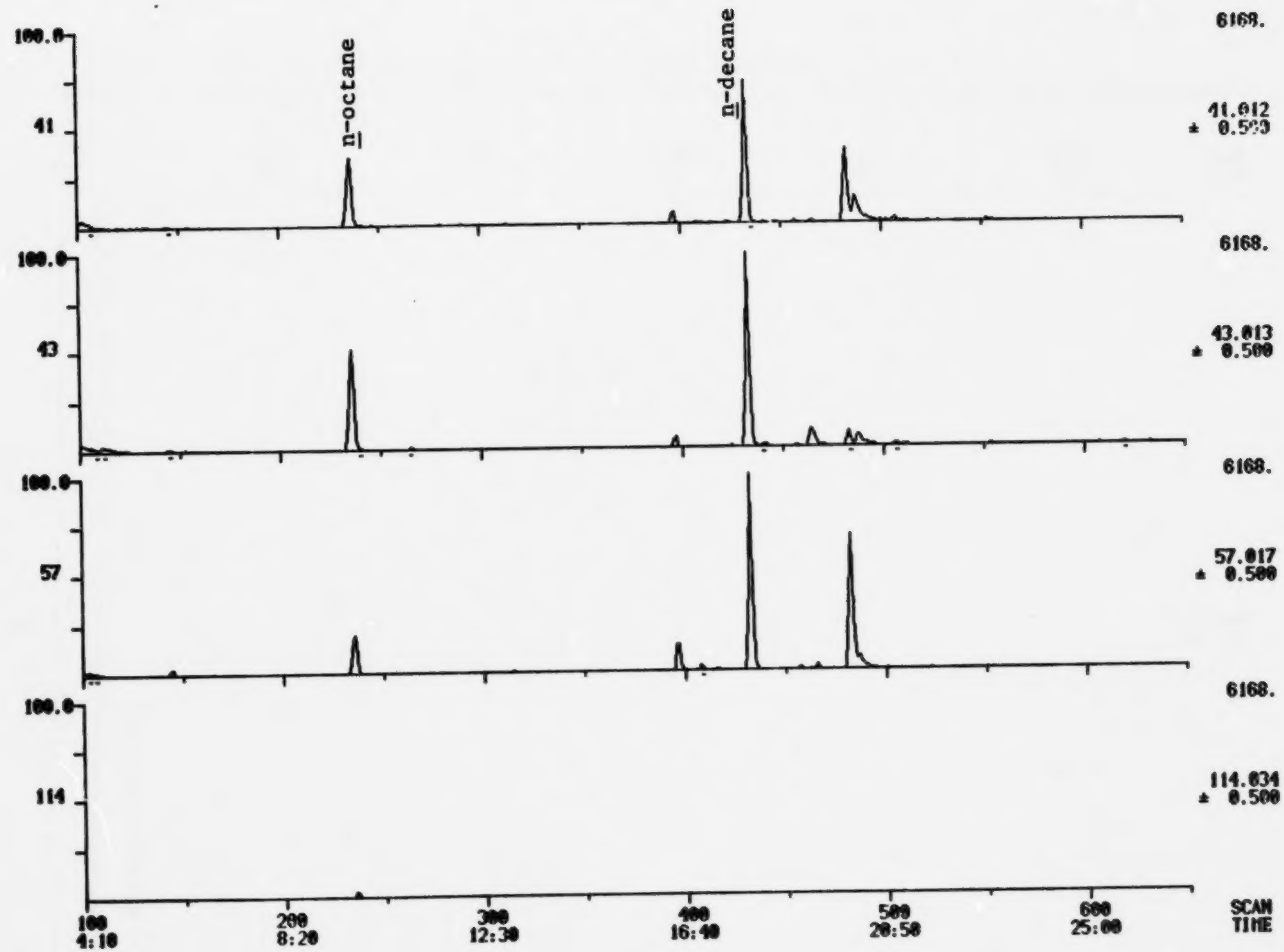


Figure 4. Extracted ion current profile of m/z 41, 43, 57 and 114 for n-octane and n-decane in performance mixture (see Fig. 1 for operating conditions).

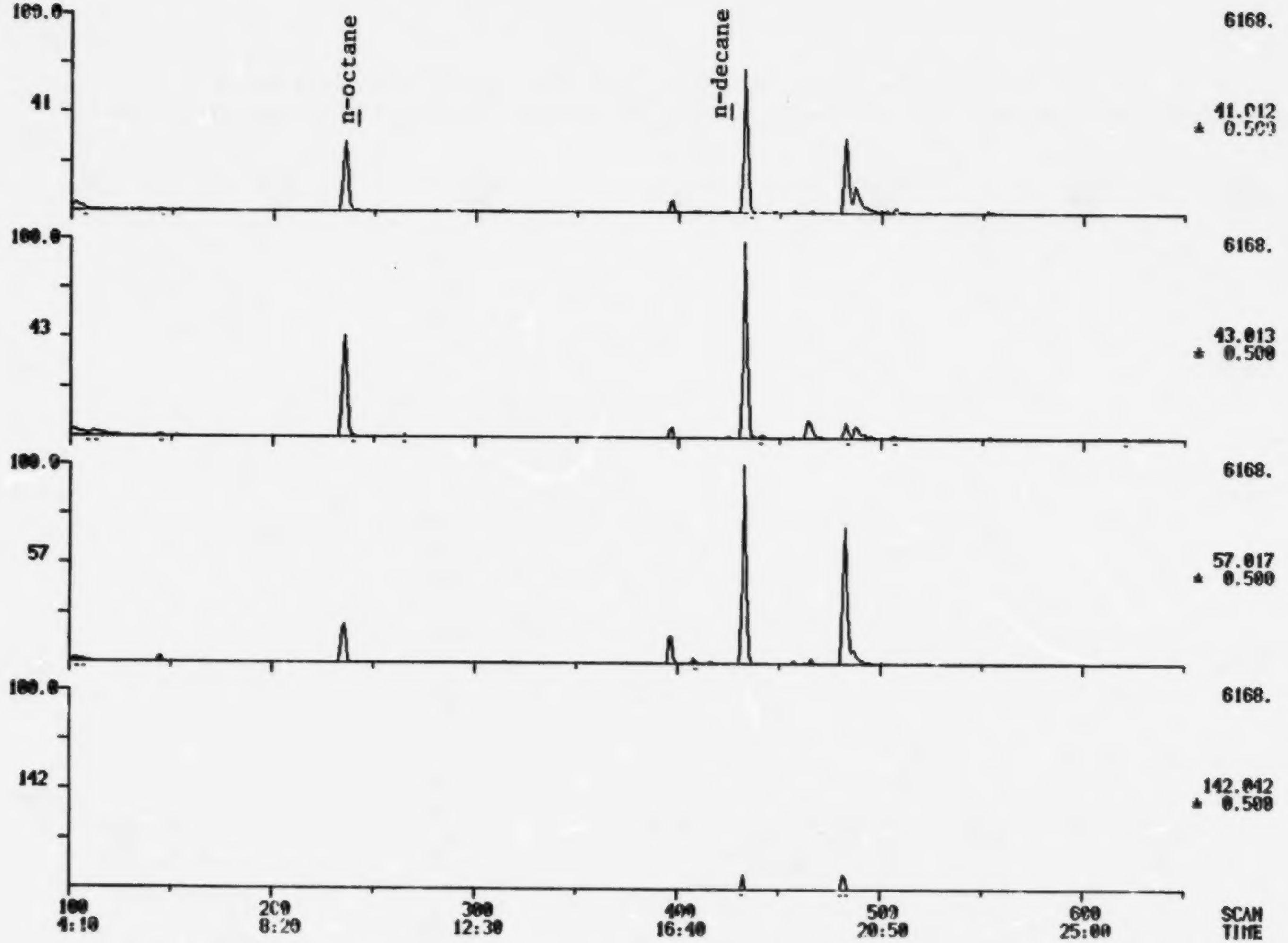


Figure 5. Extracted ion current profile of m/z 41, 43, 57, and 142 of n-octane and n-decane in performance mixture (see Fig. 1 for operating conditions).

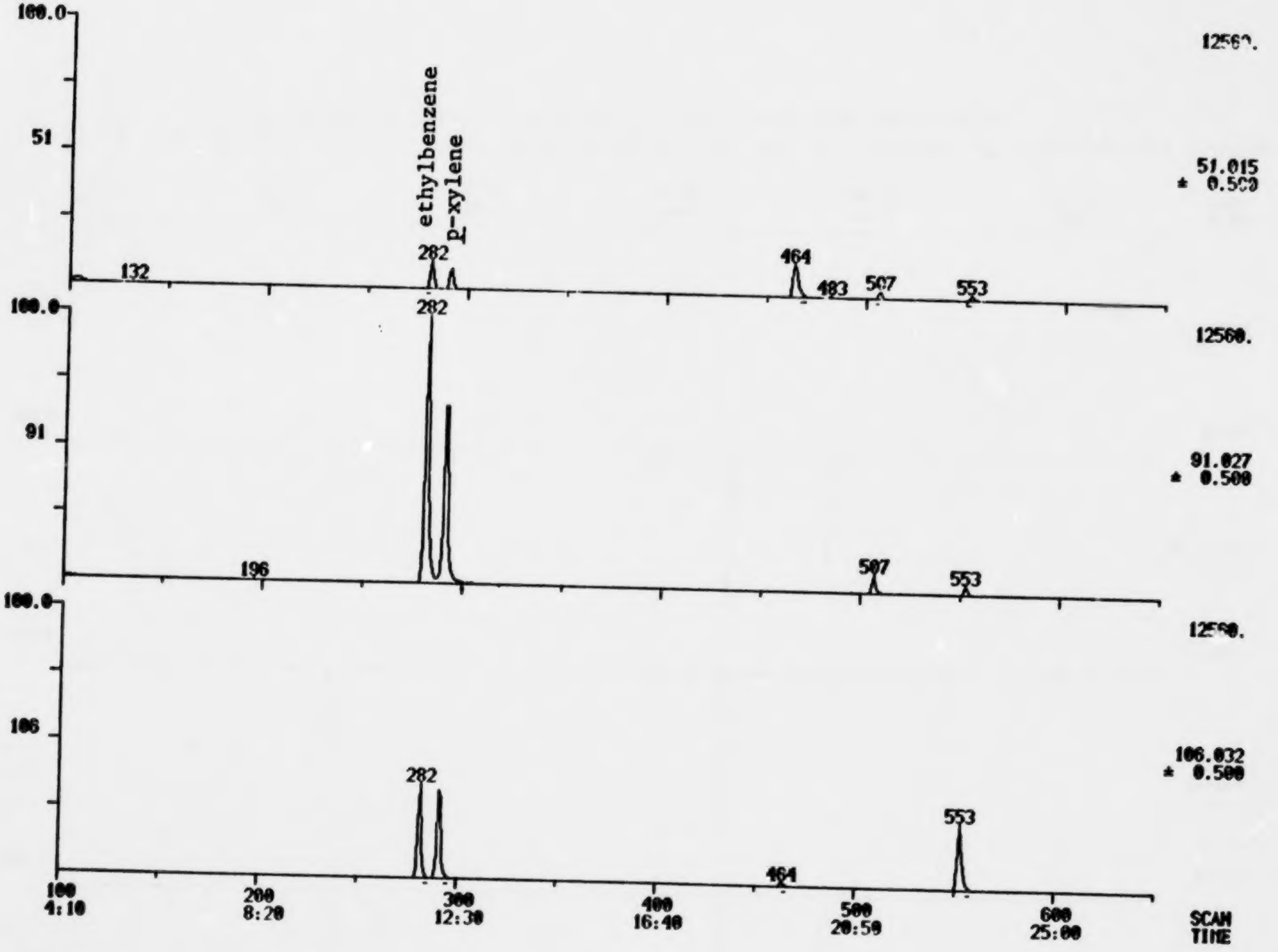


Figure 6. Extracted ion current profile of m/z 51, 81 and 106 for ethylbenzene and p-xylene in performance mixture (see Fig. 1 for operating conditions).

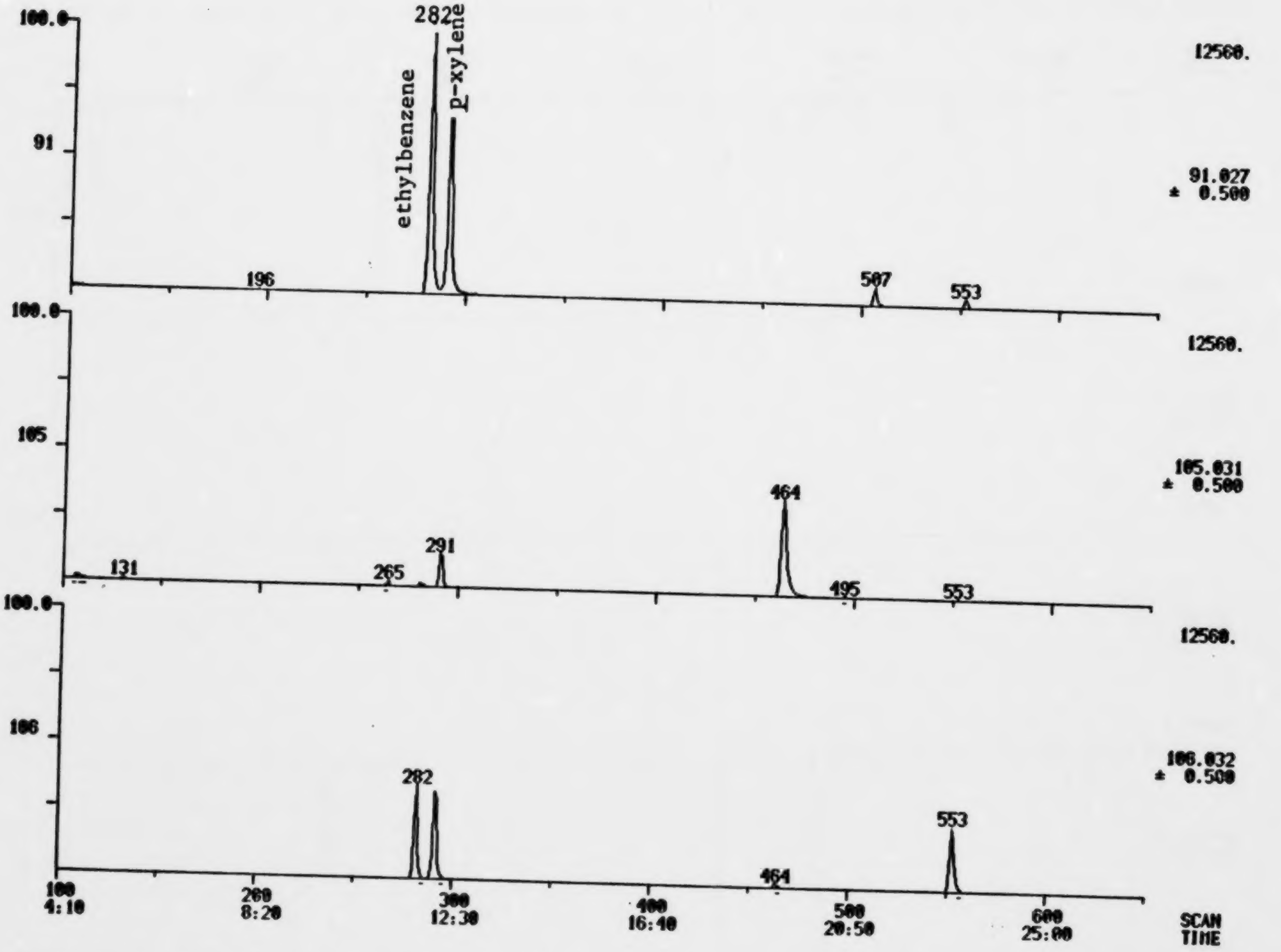


Figure 7. Extracted ion current profile of m/z 91, 105 and 107 for ethylbenzene and p-xylene in performance mixture (see Fig. 1 for operating conditions).

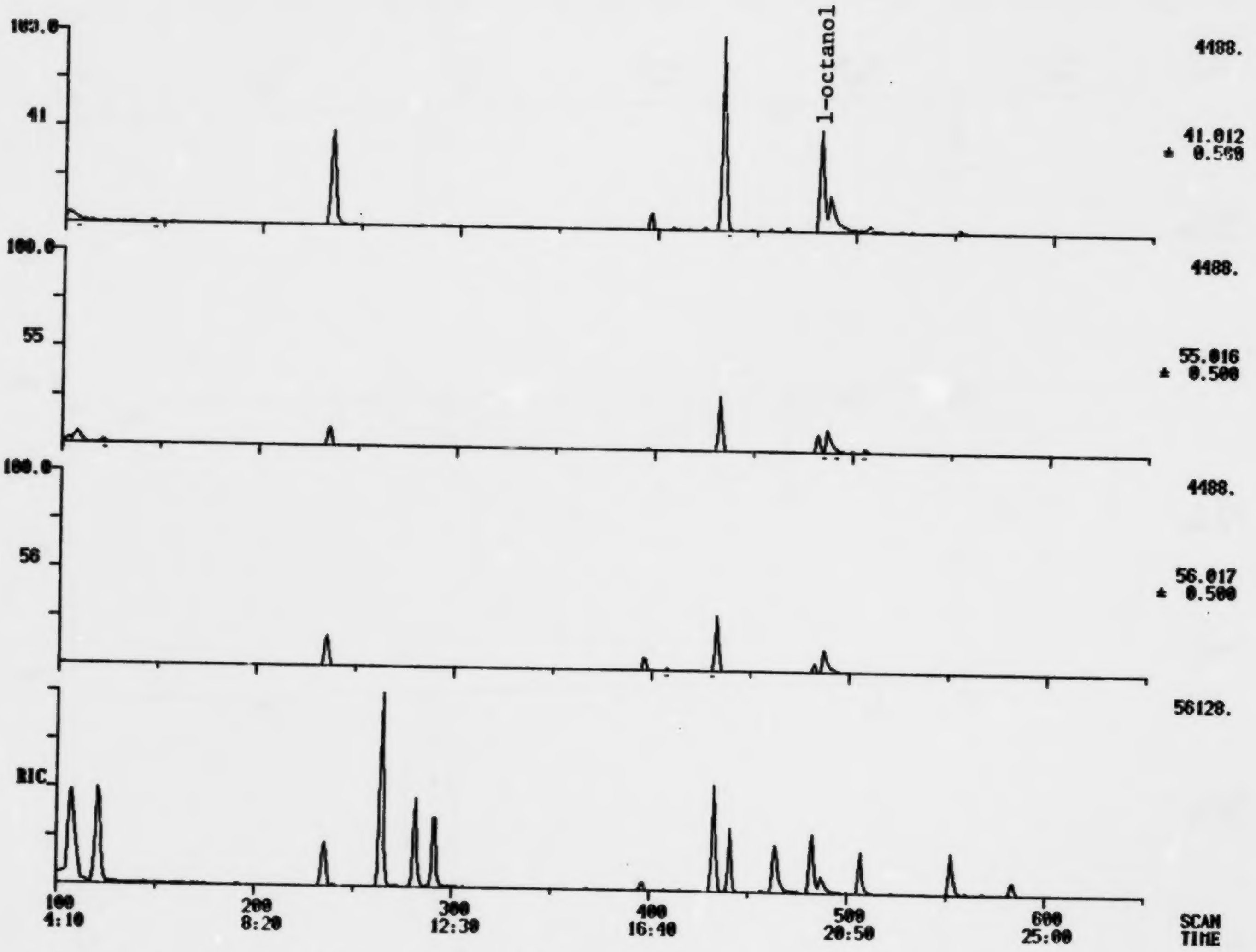


Figure 8. Extracted ion current profile of m/z 41, 55 and 56 for 1-octanol in performance mixture (see Fig. 1 for operating parameters).

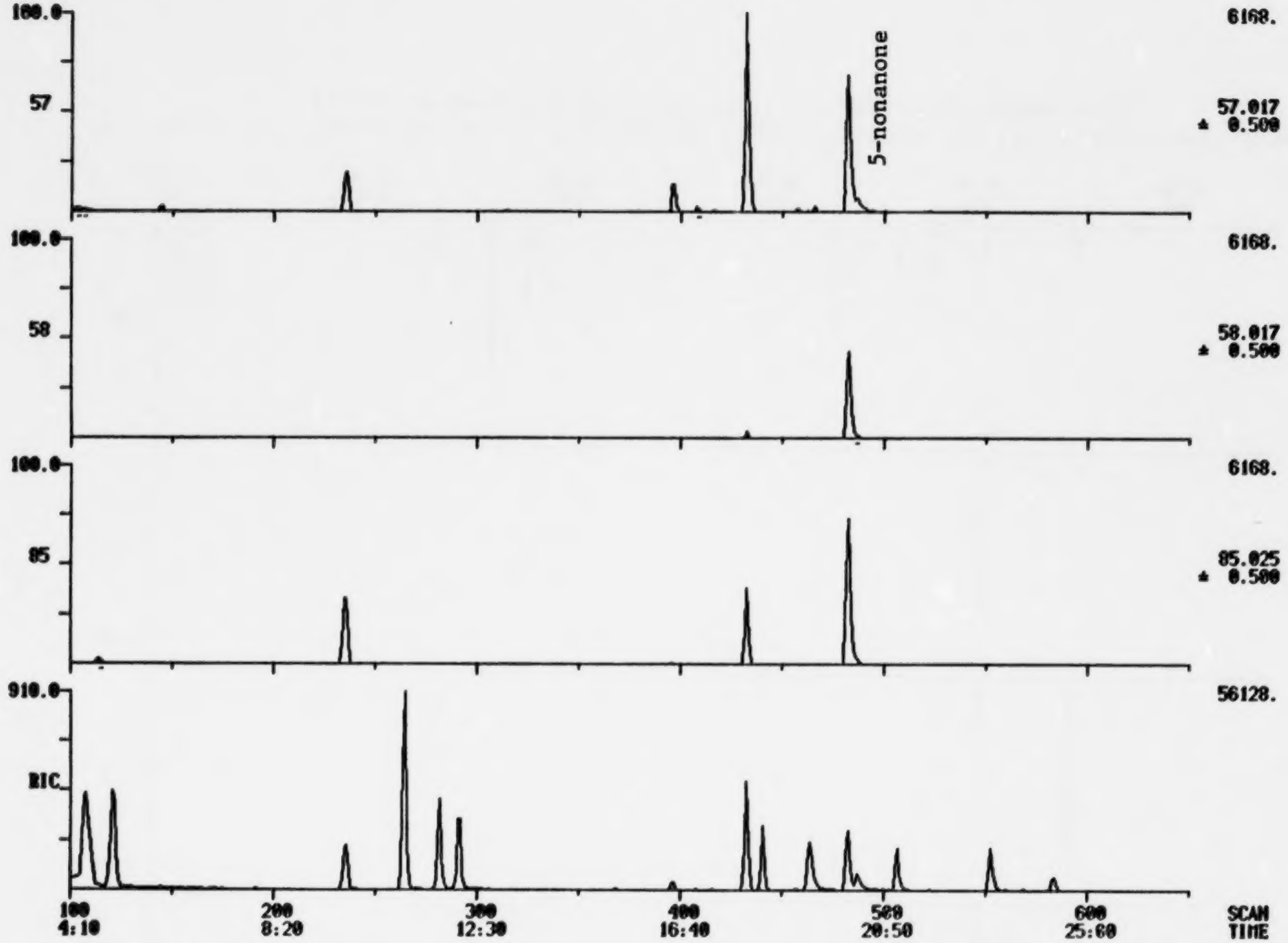


Figure 9. Extracted ion current profile of m/z 57, 58, and 85 for 5-nonanone in performance mixture (see Fig. 1 for operating parameters).

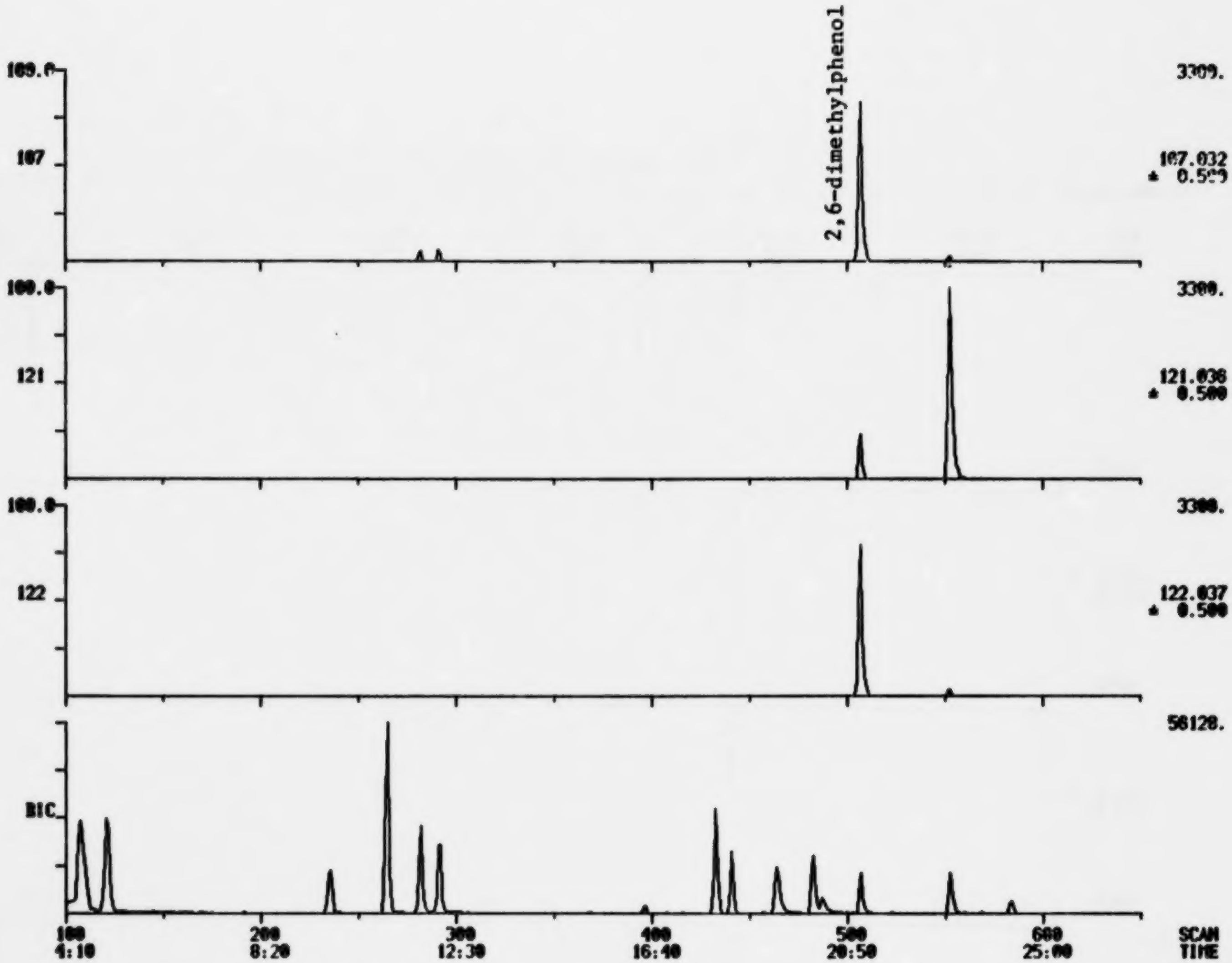


Figure 10. Extracted ion current profile of m/z 107, 121 and 122 of 2,6-dimethylphenol in performance mixture (see Fig. 1 for operating parameters).

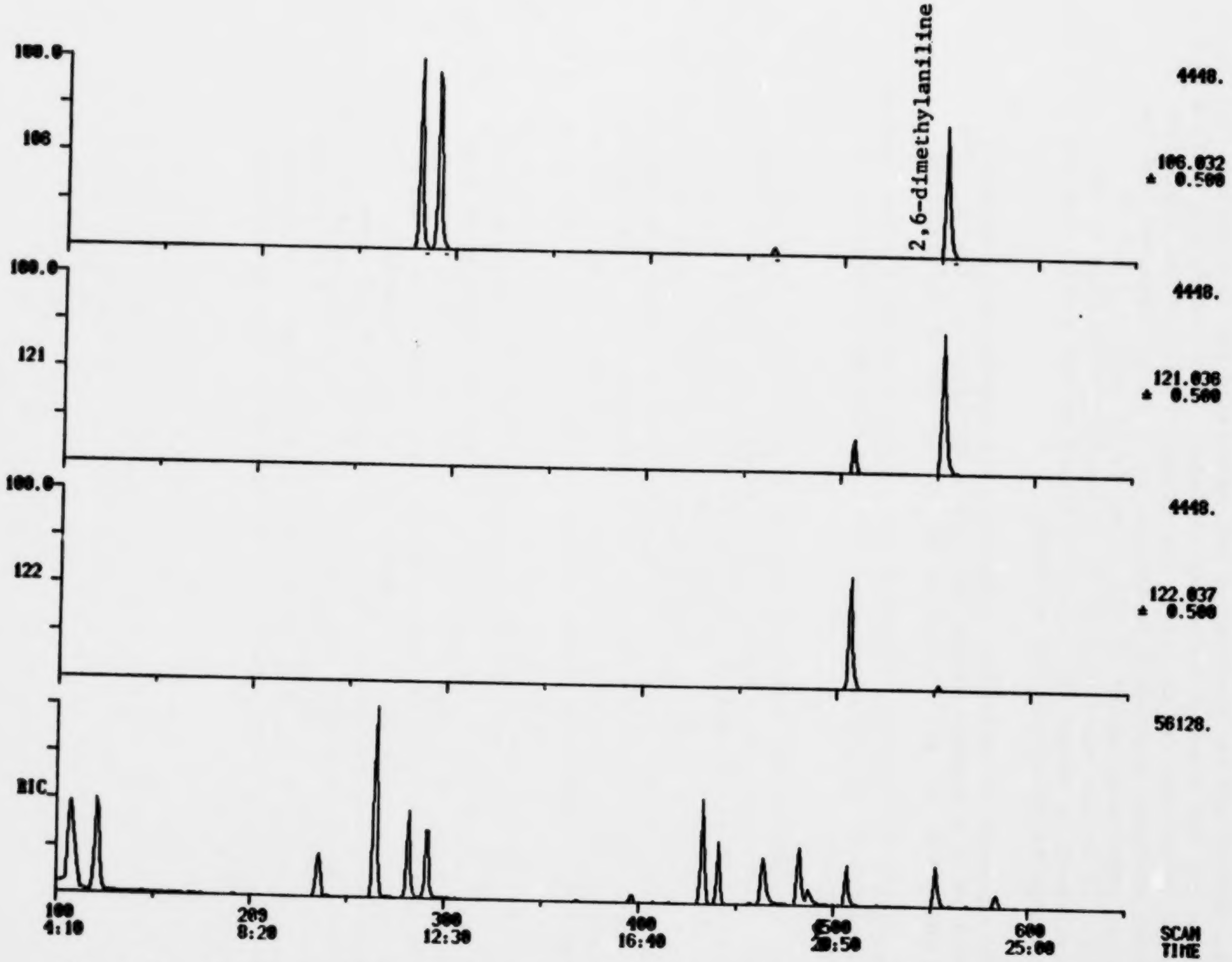


Figure 11. Extracted ion current profile of m/z 106, 121, and 122 for 2,6-dimethylaniline in performance mixture (see Fig. 1 for operating parameters).

Table 2 presents the performance obtained for a glass capillary column prepared by the barium carbonate procedure. In this case the column was 75 m in length and contained a 1 micron film thickness of SE-30. The capillary column was evaluated immediately after its preparation and continually for a period of six months and the performance was calculated for this entire period of time and the standard deviation included. A column length of 75 m has been found to be required to obtain sufficient resolution and separation of the complex mixtures obtained from ambient air. It is suggested that the resolution and separation number of the column be at least 1.3 and 70, respectively. It is the experience of this laboratory that this is the minimum requirement to obtain adequate information on the qualitative and quantitative aspects of ambient air mixtures.

For the analysis of semi-polar compounds, the percent peak asymmetry factor should be at a minimum within the ranges specified in Table 2. For more polar compounds, the performance of the column must be far superior.

Figures 12-16 provide the extracted ion current profiles for the various ions of the component in the performance mixtures used in calculating the performance criteria.

Similar evaluation was conducted for the Grob silanized type glass capillaries. The results were superior with respect to the percent asymmetry factor for these compounds and the capillaries exhibited better non-basicity characteristics. However, it is not known what the lifespan of the Grob silanized column will be under continual usage for the analysis of ambient air pollutants utilizing Tenax GC cartridges followed by thermal desorption. The barium carbonate columns deactivated using Carbowax 20M and coated with SE-30 have proven to be versatile and rugged for this application. Several columns have been prepared and have exhibited lifespans of 6-9 months.

For the purpose of maintaining quality control during the analysis of ambient air samples using the cartridge technique, it is recommended that these performance criteria be adopted and that the performance mixture be loaded onto the Tenax cartridge utilizing the flash evaporation technique described in Section 8 with the performance mixture analyzed on a daily basis. In this manner historical documentation of the performance of the entire system including thermal desorption, chromatography and transfer to the ion source can be developed and recorded. The incorporation of perfluorotoluene in the performance mixture serves the purpose of checking the mass intensity calibration of the instrument under scanning capillary chromatography. The use of perfluorotoluene for calibration of mass and intensity is dicussed in Section 8.

Table 2. PERFORMANCE OF GLASS CAPILLARY PREPARED BY BARIUM CARBONATE PROCEDURE[a]

Parameter	Test Compound(s)	Value ± S.D. (C.V.)
Resolution	Ethylbenzene:p-Xylene	1.30 ± 11 (8)
Separation No.	Octane:Decane	73 ± 6 (8)
% Peak Asymmetry Factor	1-Octanol	239 ± 141 (59)
	Nonanone	130 ± 32 (25)
	Acetophenone	260 ± 34 (13)
Acidity	2,6-Dimethylaniline:Acetophenone	1.00 ± 0.07 (9)
Basicity	2,6-Dimethylphenol:Acetophenone	0.82 ± 0.03 (5)

[a] SE-30 WCOT/$BaCO_3$, 0.48 mm i.d. x 75 m, 1 μ film thickness. Capillary had been in use for analysis of ambient air pollutants by GC/MS/COMP for six months when final evaluation was performed.

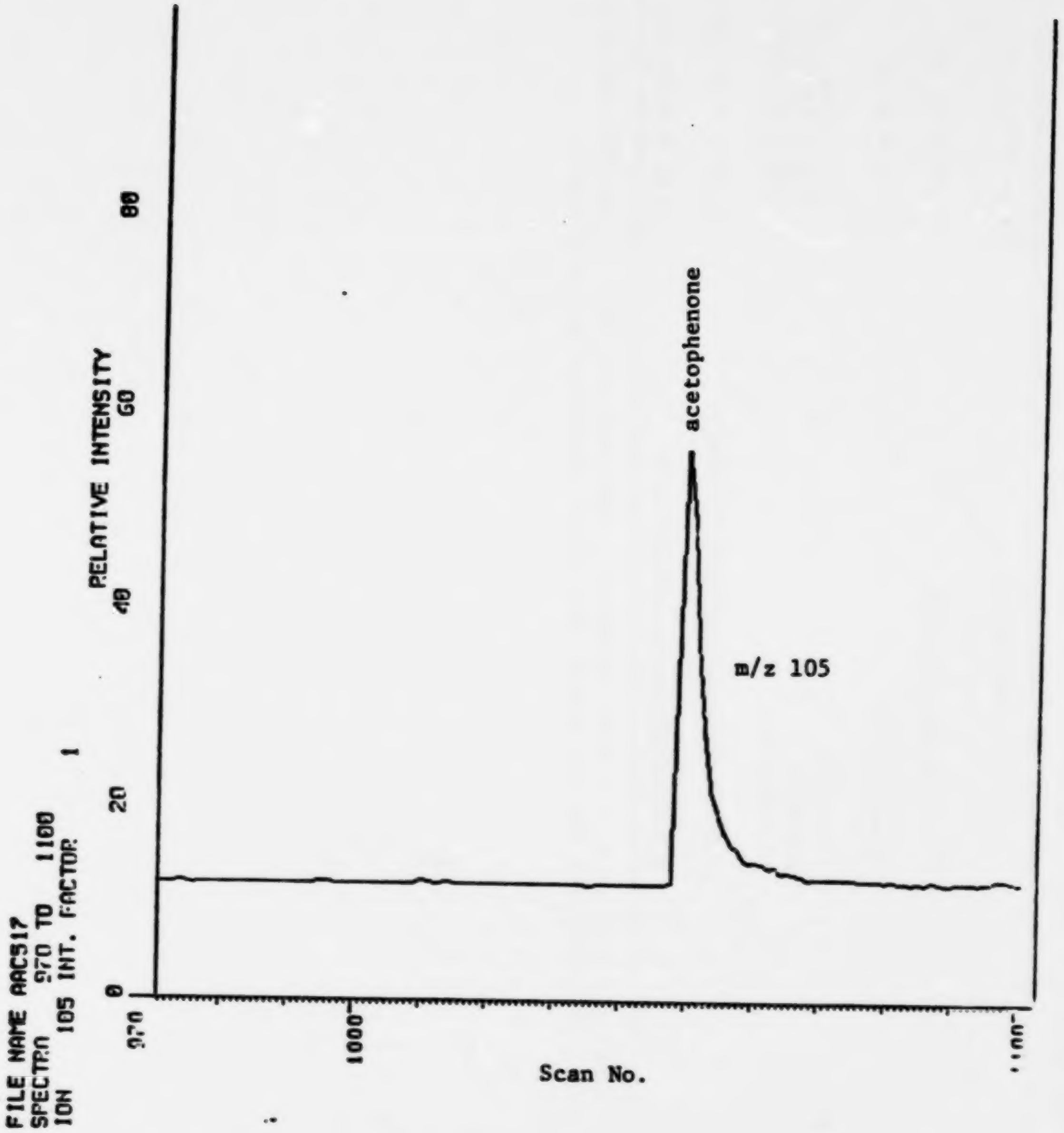


Figure 12. Extracted ion current profile of m/z 105 for acetophenone in calculating percent peak asymmetry factor.

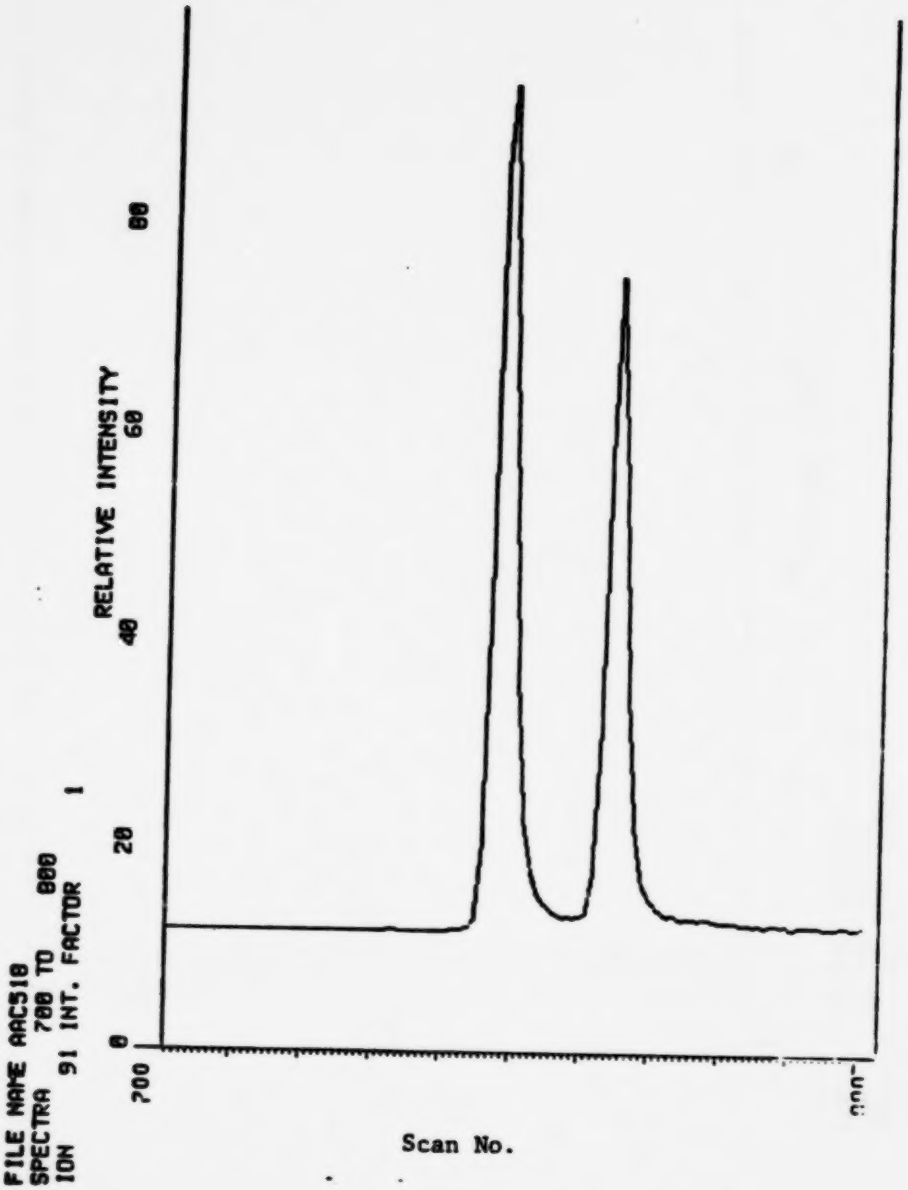


Figure 13. Extracted ion current profile of m/z 91 for p-xylene and ethylbenzene used in calculating resolution.

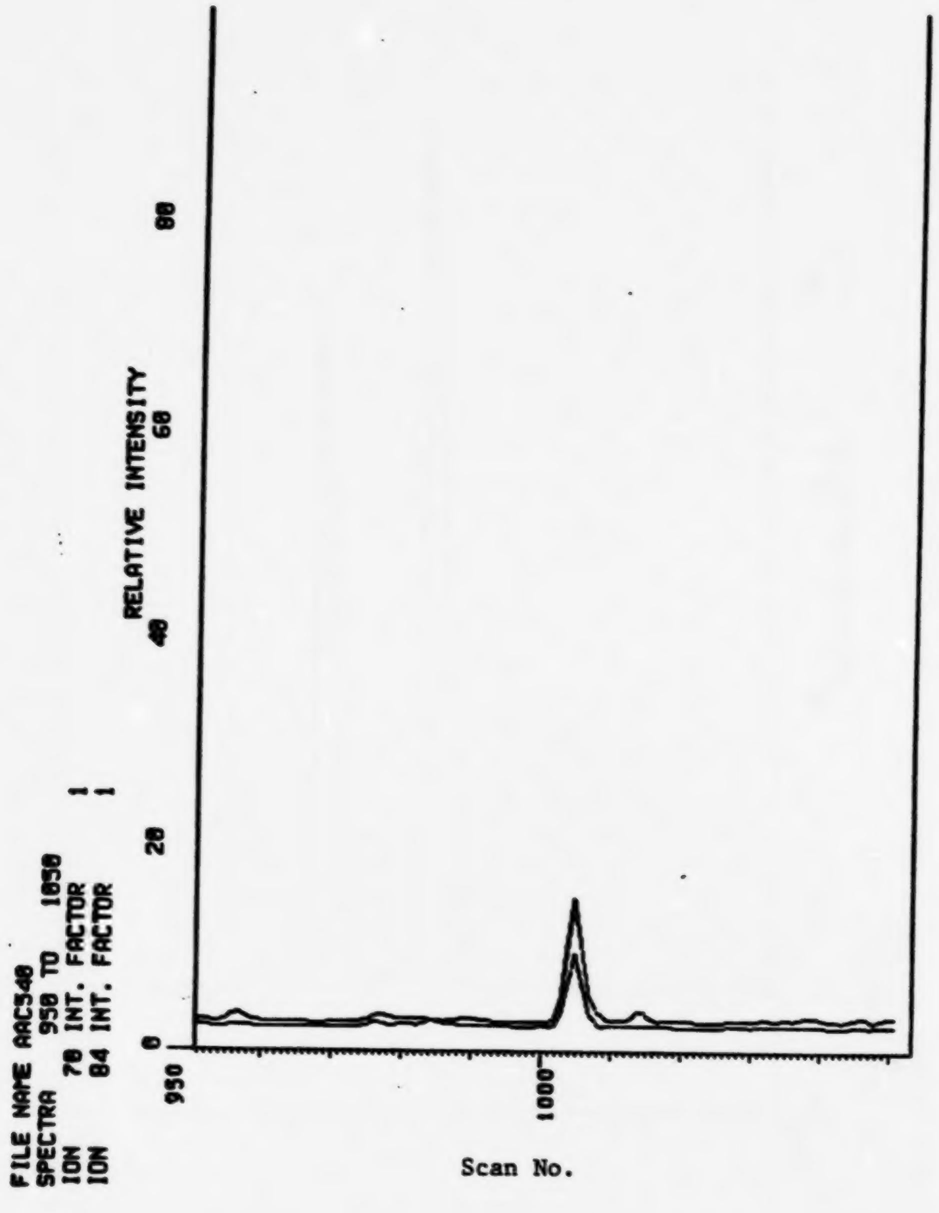


Figure 14. Extracted ion current profile of m/z 70 and 84 for 1-octanol used for calculating percent peak asymmetry factor.

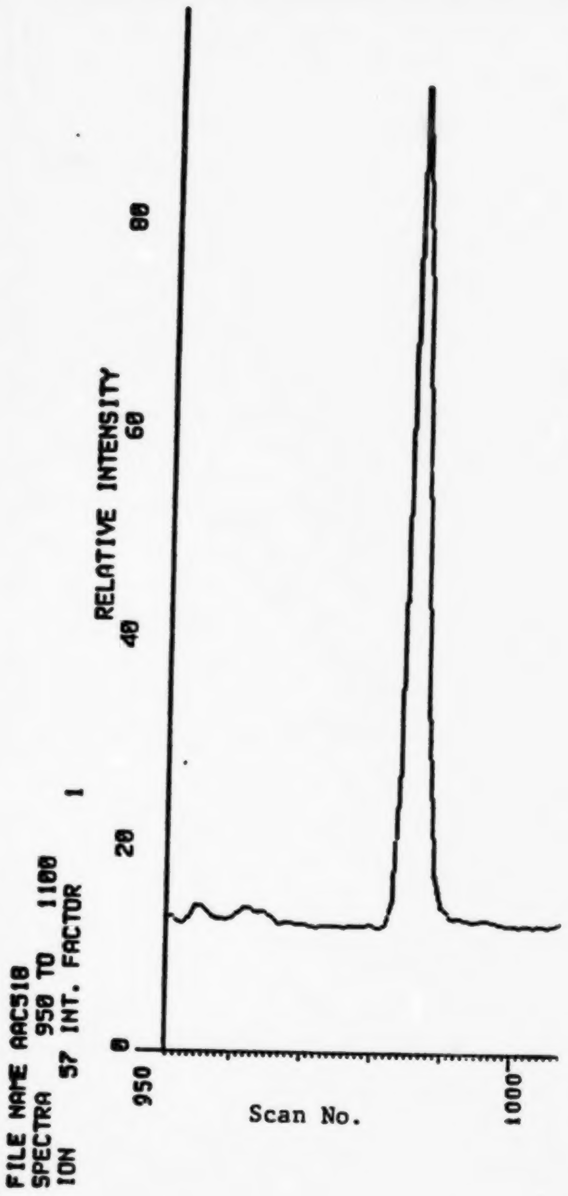


Figure 15. Extracted ion current profile of m/z 57 for nonanone used in calculating percent peak asymmetry factor.

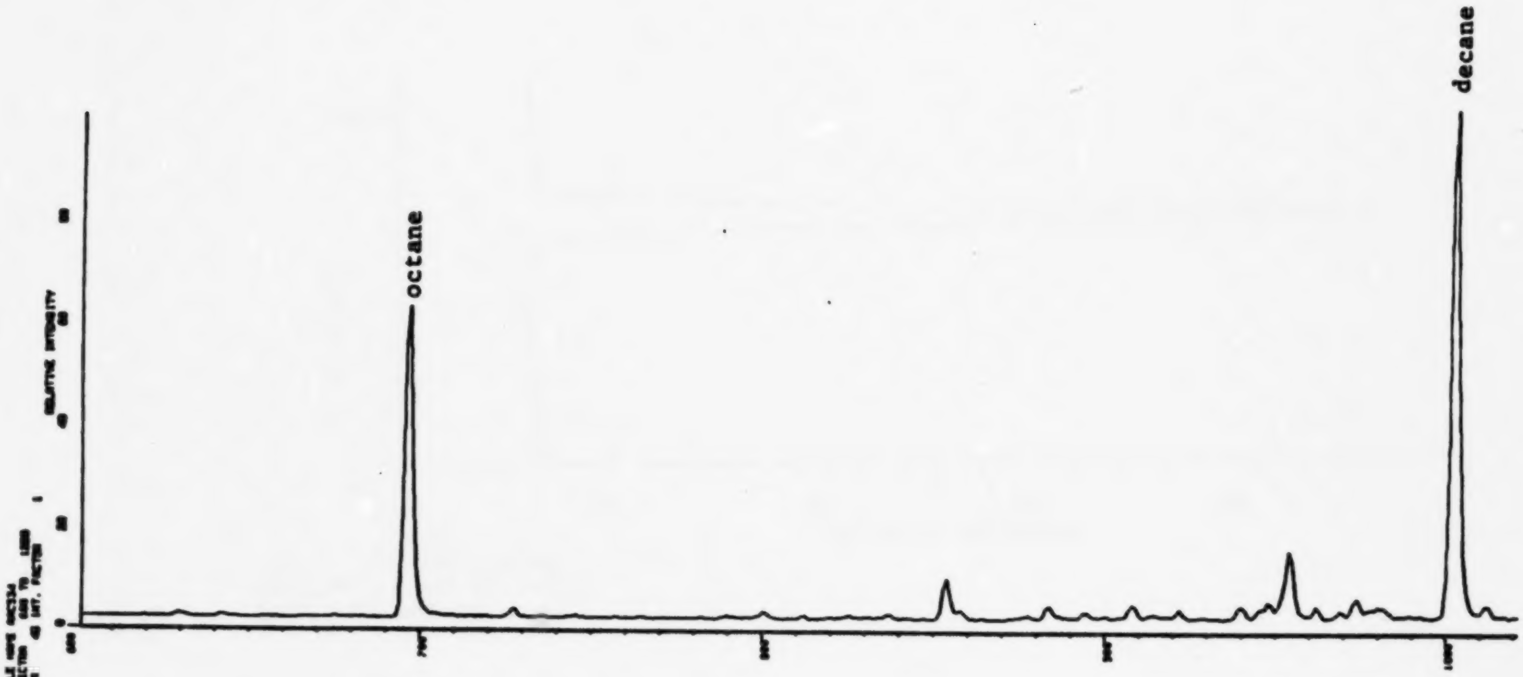


Figure 16. Extracted ion current profile of $\underline{m}/\underline{z}$ 43 for octane and decane used in calculating separation number.

SECTION 6

GAS CHROMATOGRAPHY/NEGATIVE CHEMICAL IONIZATION MASS SPECTROMETRY/ COMPUTER ANALYSIS OF AMBIENT AIR SAMPLES

INTRODUCTION

The prevalence of halogenated hydrocarbons in the environment is well documented. In ambient air alone, over 250 halocarbons have been identified by glass capillary GC/MS/computer. In a single air sample, often 10-50 halogenated hydrocarbons may be present along with the large number of other organic vapor-phase compounds. Because of their wide spread occurrence and the need for improvements in the selectivity of analysis for halogenated compounds in ambient air, the technique of negative chemical ionization mass spectrometry was investigated as a potential method for their analysis. The collection device (Tenax GC) employed in the collection of organic vapor phase compounds from ambient air is highly efficient since in a sample over 200 organic compounds are routinely detected. With the advent of an additional sorbent to collect the more volatile vapor-phase organics for which Tenax GC is not suitable, an extremely complex mixture of compounds will be presented to the GC/MS/computer system. In order to improve upon the selectivity of analysis negative chemical ionization mass spectrometry was investigated as a potential technique for halogenated compounds. Ultimately, examination of negative chemical ionization (NCI) for measuring other chemical classes through the judicious selection of reagent gases is a subject of future investigations.

Electron capture in itself is a relatively old detection mode and has been well studied. The series of potential non-dissociative and dissociative reactions which can occur between a thermal energy electron and an organic molecule possessing an appreciable electron capturing affinity has been reviewed (9). These reactions are extremely important not only to the understanding and utilization of the electron capture detector as a detector for gas chromatography, but also in NCI mass spectrometry. Whether the mechanism of electron capture is one of a dissociative or non-dissociative nature depends upon the ability of the molecules to distribute the electron charge via a resonance mechanism in the parent molecule or via resonance in a product ion. In general, molecules which undergo dissociative electron capture exhibit higher sensitivity than those which are non-dissociative. Furthermore, as one increases the temperature the sensitivity also increases for those molecules which undergo a dissociative mechanism. Conversely the temperature sensitive relationship is inversely proportional for non-dissociative type mechanisms. In this section the new technique of NCI is briefly examined as a potential tool for the selective detection of halogenated hydrocarbons. Furthermore its potential as a tool for rapidly screening for the presence of halogenated hydrocarbons in ambient air samples is presented.

MATERIALS AND METHODS

Sampling

The collection of vapor phase organics from ambient air is described under Section 8. Replicate samples which served as backup samples for those subjected to conventional electron impact capillary GC/MS/computer analysis were submitted to NCI analysis.

Instrumental Methods

An LKB Model 2091 GC/MS system was used in these studies. The mass spectrometer was equipped with a PDP/11-04 32K central processor computer system. The data system contained a dual 24 million byte disk system, nine-track Pertec IBM-compatible magnetic tape drive, a Versatec 800A printer/plotter, an operator console and a Tektronix 4012 display. The GC/MS system was equipped with a Pye-Unicam 104 gas chromatograph and a dual ionization source for electron impact (EI) and chemical ionization. A single stage Becker-Ryhage separator interfaced the GC to the mass spectrometer. Scan speeds (either parabolic or exponential) of 1-2 sec/mass decade were used.

The operational parameters for NCI GC/MS analysis are given in Table 3. The recovery of vapor-phase organics collected on Tenax GC cartridges was achieved using standard operating parameters. The chromatographic column was a 75 m glass SE-30 coated wide bore barium carbonate WCOT (Section 5).

RESULTS AND DISCUSSION

Negative chemical ionization mass spectrometry has great potential in the analysis of vapor phase organics collected from ambient air. A case example exhibiting its utility is exemplified for an ambient air sample using EI and NCI. The Tenax GC sampling cartridge was utilized to collect vapor-phase organics for the subsequent analysis by negative chemical ionization. Figure 17 depicts a GC/MS/COMP profile obtained by thermal desorption of the Tenax GC cartridge using electron impact. Well over 100 compounds were observed. However, when a corresponding duplicate sample was analyzed utilizing the same technique except for operating the mass spectrometer in the NCI mode, the results shown in Figure 18 were obtained. These results represent a sample taken upwind from an industrial area in Deer Park, TX (see Section 8). Representated are the reconstructed ion intensities for ^{35}Cl, ^{37}Cl, ^{79}Br and ^{81}Br. By noting the chromatographic peaks at specific retention times, the number and combination of chlorine and bromine atoms in a molecule are clearly evident. Figure 19 depicts a profile for an ambient air sample taken downwind from the same industrial area in Deer Park, TX. In addition to the compounds which were detected in the upwind samples, several new compounds are also detected in the downwind sample.

Table 3. OPERATING PARAMETERS FOR NEGATIVE CHEMICAL IONIZATION GLC/MS/COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	270°C
capillary trap - minimum	-195°C
maximum	+250°C
thermal desorption time	8 min
He purge rate	15 mL/min
GLC	
75 m glass SE-30 wide bore (0.47 mm) WCOT, 1 μM film thickness	4 min/40°C; 40-240°C, 4°C/min
carrier (He) flow	1.5 mL/min
separator/transfer line	250°C
MS	
scan range	*m/z* 20 → 500
ion source temperature	250°C
electron energy	50 eV
trap/box current	250 μA
reagent gas	CH_4
reagent gas pressure	4×10^{5} T
accelerating voltage	3500 V
scan interval	2.0 sec

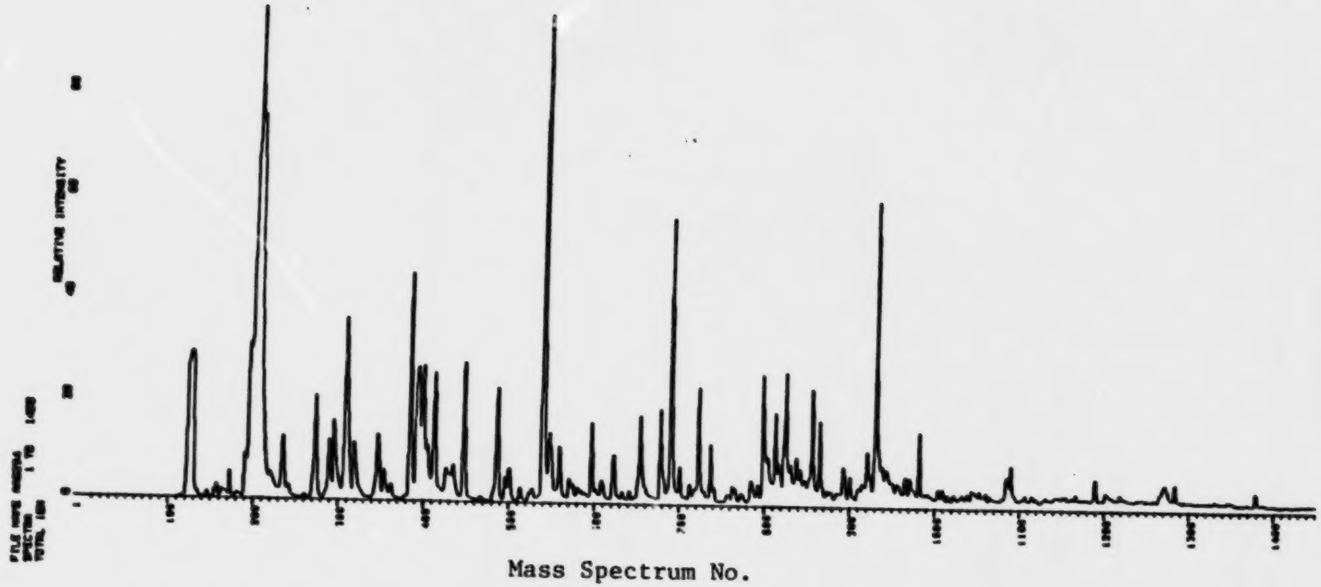


Figure 17. Electron impact GC/MS/COMP profile of vapor-phase organics in ambient air of Deer Park, TX.

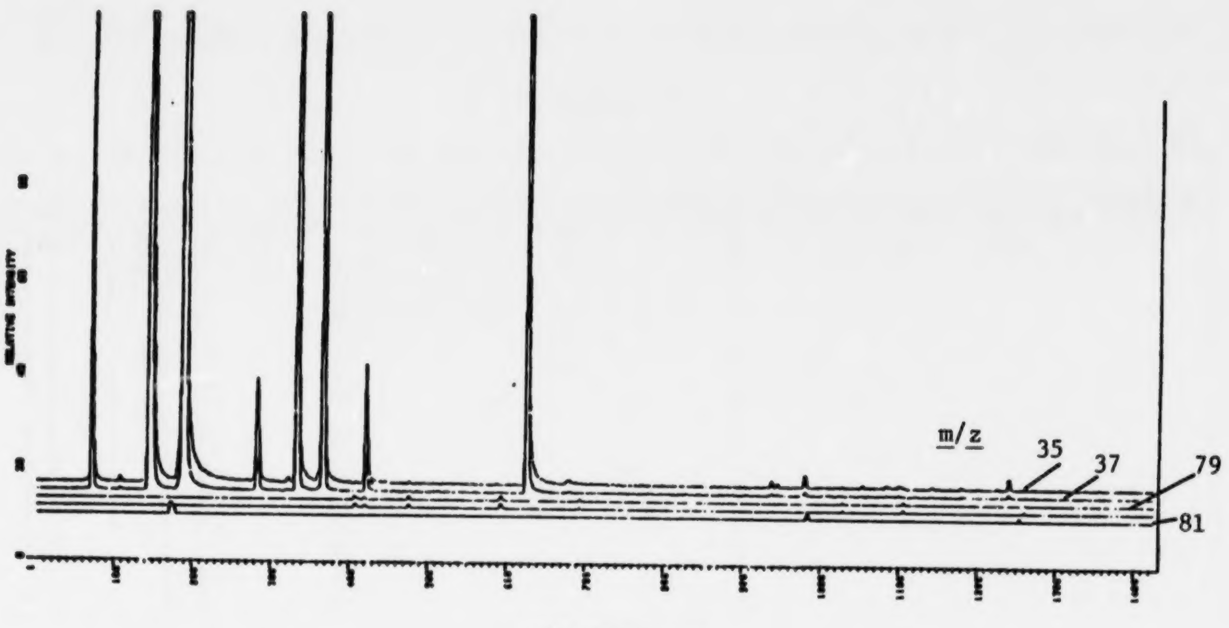


Figure 18. Negative chemical ionization GC/MS/COMP profile of upwind ambient air sample for Deer Park, TX.

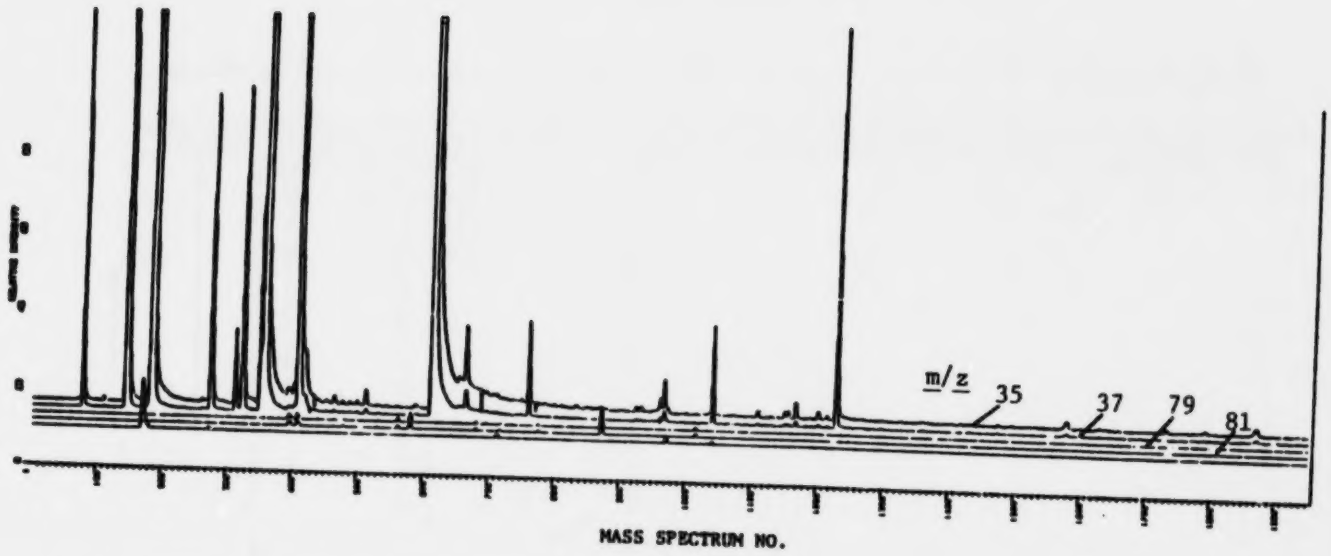


Figure 19. Negative chemical ionization GC/MS/COMP profile of downwind ambient air sample in Deer Park, TX.

The power of this technique is exemplified in the specificity and sensitivity which is not afforded in EI mode. As can be seen from these data, the intensity of each of the peaks which corresponds to halogenated hydrocarbons is much greater than in the electron impact mode. The technique is on an average of 2-3 orders of magnitude more sensitive than electron impact. Furthermore, NCI/MS provides considerable specificity which is mandatory for the analysis of vapor-phase organics in ambient air if elaborate purification methods are to be circumvented. Extensive purification of an ambient air sample is precluded by the high volatility of the compounds and severe losses would occur in the transfer step(s).

The utility of this method is apparent for the analyst who is interested in halogenated hydrocarbons in the environment. This tool is extremely beneficial for the preliminary quick screening of samples collected in a geographical area for which little information exists on the qualitative or quantitative composition of the atmosphere. By judiciously selecting samples collected surrounding a geographical area it is possible to quickly ascertain the significant halogenated compounds present by using NCI. This technique circumvents labor intensive steps which otherwise would be necessary using EI when searching for halogenated hydrocarbons in complex organic vapor-phase mixtures. A quick inspection such as exemplified by Figures 18 and 19 allows the analyst to quickly ascertain the number and magnitude of the halogenated hydrocarbons potentially present in the ambient air samples. The alternate conventional method of EI analysis requires the examination of all data generated for identification and/or detection of halogenated compounds. The level of effort necessary with this approach can be as much as 5-10 times greater than by simply analyzing a replicate sample by NCI and reconstructing the $\underline{m}/\underline{z}$ isotopic profiles for chlorine, bromine, iodine and fluorine.

This technique was also applied to studies on in situ reactions occurring between molecular halogens and organic vapors collected on Tenax GC XAD-4 and charcoal sorbents (see Section 7).

In summary, the technique of capillary GC/NCIMS/COMP analysis of vapor-phase organics offers a considerably faster method for detecting and for potentially quantifying electron capturing substances present in ambient air samples. This serves as an improvement in the basic GC/MS/COMP analysis of vapor-phase organics in air and its full potential use for this type of analysis still awaits full exploitation.

SECTION 7

IN SITU REACTION STUDIES ON SORBENTS USED FOR COLLECTION OF VAPOR-PHASE ORGANICS

INTRODUCTION

In previous reports, the detection, identification, and quantitation of halogenated hydrocarbons in the ambient air have been described. Ambient air was sampled using a Tenax GC cartridge technique and sample analysis employed high resolution (glass capillary) gas chromatography/mass spectrometry/computer (HRGC/MS/COMP) methods. Since the beginning of the development of this technique over 7 years ago, many halogenated hydrocarbons have been identified and quantified in ambient air from several geographical regions throughout the Continental U.S.

In view of the potency in the broad spectrum of the carcinogenic activity (in experimental animals) for the halogenated hydrocarbons identified, the detection of these compounds in the atmosphere has generated considerable interest in their origin. Previous studies were initiated to determine emission of halogenated hydrocarbons from stationary and fugitive sources as well as their potential formation through photochemical reactions.

In order to determine whether halogenated hydrocarbons may be present in the atmosphere from industrial sources or as products of atmospheric chemical reactions, it is first necessary to know the extent to which these compounds may form at trace levels as an "artifact" of the technique employed or the sample collection process.

The primary concern has been with the use of the Tenax GC sampling cartridge which has been extensively employed for collecting organic vapor from ambient air for characterization and quantification purposes. Since the Tenax GC cartridge may concentrate reactive compounds, including ozone, NO_x and, for example, molecular chlorine or bromine, in situ formation of artifact compounds may occur even though inorganic gases do not appreciably accumulate on the sorbent. Thus the purpose of this study was to further supplement previously reported observations, i.e., the in situ formation of nitrosoamines and to determine whether other additional in situ reactions could occur on the Tenax GC sampling cartridge under field sampling conditions.

Because urban air often contains substantial concentrations of ozone and NO_x, a limited number of laboratory experiments and to a greater extent field experiments were performed to determine whether air containing these gases might be more effective than air containing only olefins plus molecular halogens. Experiments were designed to delineate the transformation of olefins (whether adsorbed on sorbents or occurring in air) via homogeneous or heterogeneous reactions which might take place on the walls of the sample inlet tube or the sorbent bed itself. In addition to the halogenation of olefins (endogenous or exogenous in air) the possibility of reactions between ozone and these olefins producing polar products to be considered as artifacts of the collection process was investigated.

EXPERIMENTAL

Apparatus For Laboratory Studies

The apparatus used to determine whether air containing ozone, olefins and water might convert olefins to oxygenated products on Tenax GC (35/60 mesh, Applied Science Lab., State College, PA) is depicted in Figure 20. Ozone was generated by an ultraviolet lamp equipped with a sliding cover for obtaining different concentrations. The concentration of ozone was measured using a Bendix Ozone Analyzer. The intake for this instrument was at the same point as the intake for the Tenax GC glass cartridge sampler (6.0 cm bed length x 1.5 cm i.d.) through which air was drawn by a Nutech Model 221A (Nutech, Durham, NC) sampler. The sampling cartridge and the analyzer inlet tube were centered in the air flow pattern from the reaction tube. Various levels of relative humidity in the air stream were produced by changing the temperature of the humidifier bath.

Perdeuterated toluene and styrene were introduced to a Tenax GC sampling cartridge as a discrete band at one end of the sorbent bed. An air stream containing ozone (200 ppb) was sampled. Control cartridges consisted of a blank (no deuterated compound) and deuterated compounds loaded onto Tenax GC cartridges which were analyzed without exposure to ozone.

Preparation of Sorbent Cartridges

Prior to its use, Tenax GC was purified by Soxhlet extraction for 18 h with methanol and n-pentane, respectively. After drying in a N_2 atmosphere, Tenax GC was heated to 150°C for 2 h in a vacuum oven (12" of water), sized into a 35/60 range and packed into glass tubes (6.0 cm bed length x 1.5 cm i.d.). All sample cartridges were preconditioned by heating to 275°C for 20 min under a helium purge of 20-30 mL/min. While cooling in precleaned Kimax® culture tubes, the containers were sealed to prevent contamination of the cartridge.

Sample Analyses

HRGC/EI/MS--

A Varian MAT CH-7 GC/MS with a 620 L computer system equipped with an inlet manifold was used for analyzing Tenax GC cartridges where structural confirmation was required. The software programs available with this system provide reconstructed gas chromatograms and extracted ion current profiles for correlation between mass spectrum number and retention time. Operating parameters for the HRGC/MS/COMP system are given in Table 4. A single stage

Table 4. OPERATING PARAMETERS FOR GC ELECTRON IMPACT MS/COMP SYSTEM

Parameter	Setting
Inlet-manifold	
thermal desorption chamber	270°C
valve	270°C
cryo-focusing capillary trap - minimum	-195°C
maximum	+250°C
desorption time	8 min
GC	
75 m SE-30 $BaCO_3$ WCOT (0.47 mm i.d.)	30-240°C, 4°C/min
He carrier flow	1.5 mL/min
separator/transfer line	245°C
MS	
scan range	*m*/*z* 20-500
scan, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	4.5
ion source vacuum	*ca*. 4 x 10^{6} T

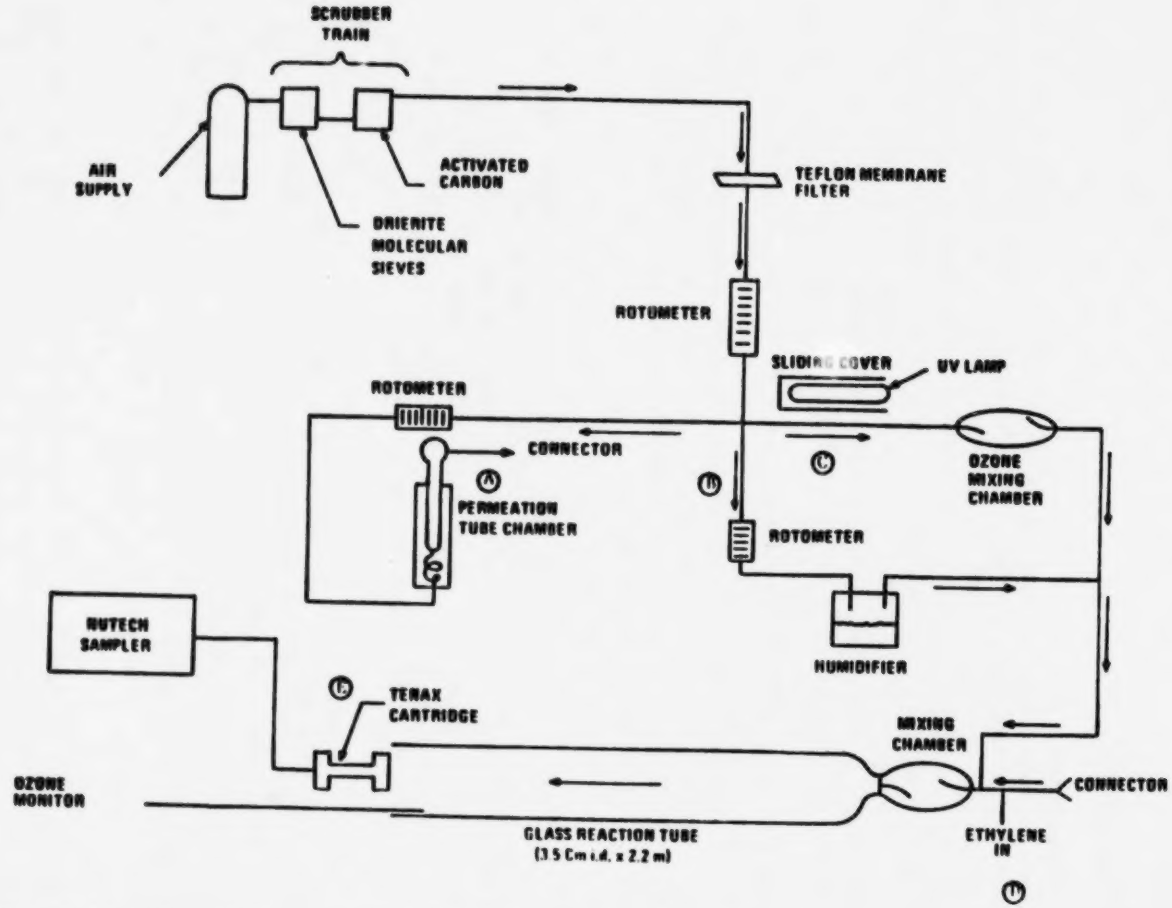

SCRUBBER TRAIN
AIR SUPPLY
ACTIVATED CARBON
DRIERITE MOLECULAR SIEVES
TEFLON MEMBRANE FILTER
ROTOMETER
SLIDING COVER
UV LAMP
ROTOMETER
CONNECTOR
Ⓐ
PERMEATION TUBE CHAMBER
Ⓑ
Ⓒ
OZONE MIXING CHAMBER
ROTOMETER
HUMIDIFIER
NUTECH SAMPLER
Ⓔ
TENAX CARTRIDGE
MIXING CHAMBER
CONNECTOR
OZONE MONITOR
GLASS REACTION TUBE (3.5 Cm i.d. x 2.2 m)
ETHYLENE IN
Ⓓ

Figure 20. Schematic of instrumentation and devices for examining in situ formation of oxygenated compounds on solid sorbents.

glass jet separator interfaced the SE-30 wide bore $BaCO_3$ WCOT capillary (Section 5) to the mass spectrometer.

HRGC/NCI MS/COMP--

Samples generated from laboratory and field in situ reaction studies were analyzed by HRGC/NCIMS/COMP using the operating parameters previously described (Section 6).

Field Sampling Experiments

Baton Rouge and Plaquemine, LA--

Field artifact studies were conducted in Baton Rouge, LA and vicinity. Table 5 presents the experimental design. A schematic of the configurations under examination in the artifact study is given in Figure 21. In this study we examined the potential bromination, chlorination and nitrosation of endogenous atmospheric organics by employing a tandem arrangement (configuration A, Fig. 21). Ambient air (~120 L) was pulled through the glass fiber filters and glass tubes followed by a cartridge containing the adsorbent, Tenax GC. The glass tube designated as T_2 contained a permeation tube of either bromine ($\sim 4 \times 10^{-7}$ g/min), chlorine ($\sim 1 \times 10^{-6}$ g/min) or dimethylamine-d_6 (7×10^{-7} g/min). Thus, molecular halogen or dimethylamine-d_6 which permeated at constant rates provided a constant sparging of the atmosphere just prior to the adsorbent. The corresponding parallel arrangement served as a control (T_1). By examining independently the cartridges labeled AD and AD_2, it was possible to differentiate endogenous compounds from those which were formed as an in situ reaction.

Lake Charles, LA--

A more in-depth study was performed on in situ reactions under field sampling conditions and this experimental design is given in Table 6. In contrast to the studies which were conducted in Baton Rouge, this study incorporated a second configuration (configuration B, Fig. 21) as well as the comparison of treated ($Na_2S_2O_3$) and untreated glass fiber filters, and teflon filters for the occurrence of in situ reactions.

Houston, TX--

Table 7 presents the experimental design for the field in situ reaction studies conducted in Houston, TX. This study was repeated to provide a greater diversity of industrial atmospheres while determining the effect of molecular halogen on the endogenous hydrocarbon background present in the atmosphere. Also, cyclohexene-d_{10} and styrene-d_8 (~1 μg each) were added to Tenax cartridges prior to samples as a discrete band at one end of the sampling bed.

Raleigh, NC--

Figure 22 presents the experimental configuration for sparging atmosphere near a major interstate with halogenated compounds and deuterated substances with the collection of the potential products by using Tenax GC sampling cartridges. Table 8 gives the experimental design for this field study.

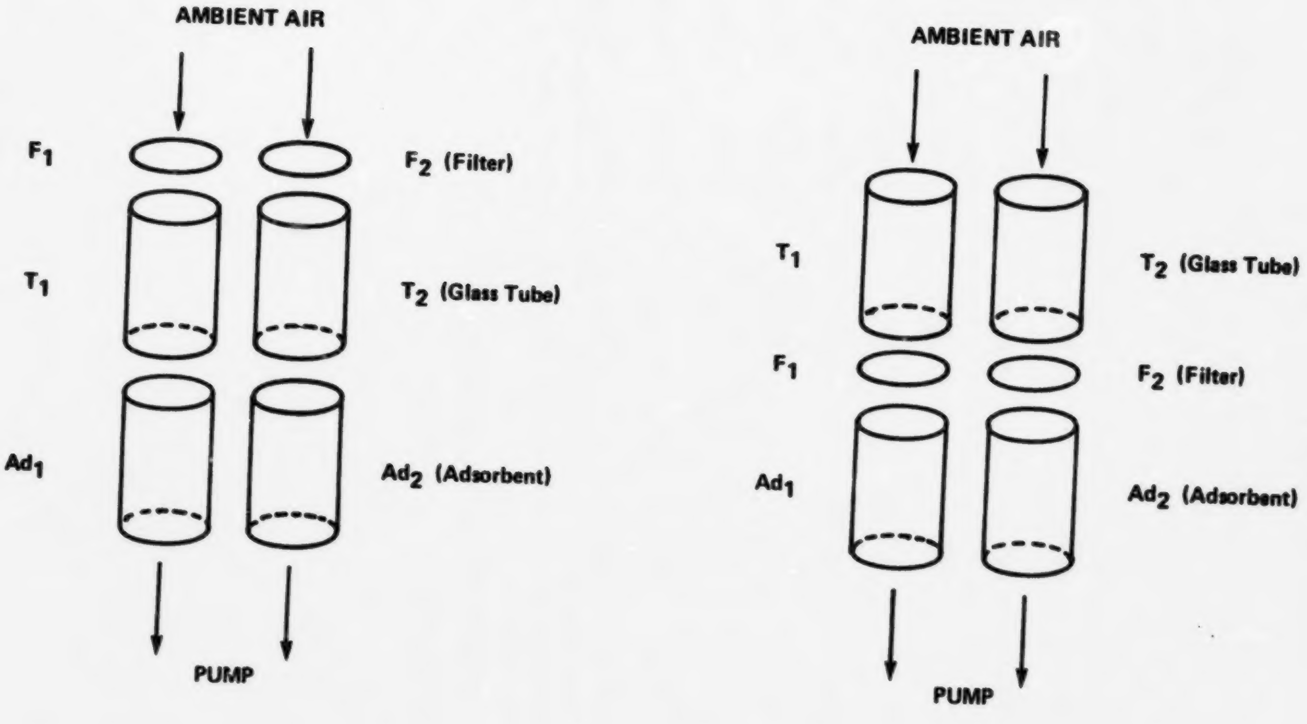
Table 5. EXPERIMENTAL DESIGN FOR FIELD *IN SITU* REACTION STUDIES IN BATON ROUGE, LA[a]

	Filter		Glass tube		Adsorbent	
Sample Code	F_1	F_2	T	T_2	Ad_1	Ad_2
P1/L5A-1	GFF-U[c]	GFF-U	-	+ Br_2	Tenax	Tenax
P1/L5A-2	GFF-U	GFF-U	-	+ Cl_2	Tenax	Tenax
P1/L5B	GFF-U	GFF-U	-	+ DMA-d_6	Tenax	Tenax
P2/L5A	GFF-U	GFF-U	-	+ Br_2	Tenax	Tenax
P2/L5B	GFF-U	GFF-U	-	+ Cl_2	Tenax	Tenax
P2/L5C	GFF-U	GFF-U	-	+ DMA-d_6	Tenax	Tenax
P3/L5A	GFF-U	GFF-U	-	+ Br_2	Tenax	Tenax
P3/L5B	GFF-U	GFF-U	-	+ Cl_2	Tenax	Tenax
P3/L5C	GFF-U	GFF-U	-	+ DMA-d_6	Tenax	Tenax

[a] See Table 42 and Figures 27 and 28 for sampling protocol and locations, respectively.

[b] Experimental configuration given in Figure 21.

[c] GFF-U = glass fiber filter, untreated.


AMBIENT AIR
F_1
F_2 (Filter)
T_1
T_2 (Glass Tube)
Ad_1
Ad_2 (Adsorbent)
PUMP
AMBIENT AIR
T_1
T_2 (Glass Tube)
F_1
F_2 (Filter)
Ad_1
Ad_2 (Adsorbent)
PUMP

CONFIGURATION A

CONFIGURATION B

Figure 21. Experimental sampling cartridge configurations for in situ reaction studies.

Table 6. EXPERIMENTAL DESIGN FOR FIELD IN SITU REACTION STUDIES CONDUCTED IN LAKE CHARLES, LA[a]

Sample Code	Experimental Configuration[b]	Filter				Glass Tube				Adsorbent			
		F_1	F_2	F_3	F_4	T_1	T_2	T_3	T_4	AD_1	AD_2	AD_3	AD_4
P1/L1	A	GFF-U[c]	GFF-U	GFF-U	GFF-U	$+Cl_2$	-	$+Br_2$	-	Tenax	Tenax	Tenax	Tenax
	B	-	-	-	GFF-U	-	-	-	$+Br_2$	-	-	-	Tenax
P3/L1	A	TF-U	-	TF-U	-	-	$+Br_2$	-	-	Tenax	-	Tenax	-
	B1	GFF-U	GFF-U	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-
	B2	TF-U	TF-U	-	-	-	$+Br_2$	-	-	Tenax	Tenax	-	-
P4/L1	A1	TF-U	TF-U	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-
	A2	GFF-T	-	GFF-T	-	-	-	$+Br_2$	-	Tenax	-	Tenax	-
	B	GFF-T	GFF-T	-	-	-	$+Br_2$	-	-	Tenax	Tenax	-	-
P5/L1	B1	TF-U	TF-U	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-
	B2	TF-T	TF-T	-	-	-	$+Br_2$	-	-	Tenax	Tenax	-	-
	A	TF-T	-	TF-T	-	-	-	$+Br_2$	-	Tenax	-	Tenax	-
P6/L1	B	GFF-U	GFF-U	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-
P8/L1	A	GFF-T	GFF-T	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-
P9/L1	A	TF-T	TF-T	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-
P10/L1	B	TF-T	TF-T	-	-	-	$+Cl_2$	-	-	Tenax	Tenax	-	-

[a] See Table 43 for sampling protocol.

[b] Experimental configurations were given in Fig. 21.

[c] GFF-U = glass fiber filter, untreated, and GFF-T indicates filter treated with 10% solution of $Na_2S_2O_3$. Likewise, TF-U, TF-T are untreated and treated Teflon filters.

Table 7. EXPERIMENTAL DESIGN FOR FIELD IN SITU REACTION STUDIES CONDUCTED IN HOUSTON, TX[a]

Sample Code	Experimental Configuration[b]	Filter				Glass tube				Adsorbent			
		F_1	F_2	F_3	F_4	T_1	T_2	T_3	T_4	AD_1	AD_2	AD_3	AD_4
P1/L1	A	GFF-U	GFF-T	GFF-U	GFF-T	$+Cl_2$	$+Cl_2$	$+Br_2$	$+Br_2$	Tenax	Tenax	Tenax	Tenax
P2/L1	A	GFF-U	GFF-T	GFF-U	GFF-T	$+Br_2$	$+Br_2$	$+Cl_2$	-	Tenax	Tenax	Tenax	Tenax
P3/L1	A	GFF-U	GFF-T	GFF-T	GFF-U	$+Br_2$	$+Br_2$	$+Cl_2$	-	Tenax	Tenax	Tenax	Tenax
P4/L1	A	GFF-T	GFF-U	GFF-U	GFF-U	$+Br_2$	$+Br_2$	$+Cl_2$	-	Tenax	Tenax	Tenax	Tenax
P5/L1	A	GFF-T	GFF-U	GFF-U	GFF-U	$+Cl_2$	-	-	-	Tenax	Tenax	Tenax	Tenax
P6/L1	A	GFF-T	GFF-U	-	-	$+Cl_2$	-	-	-	Tenax	Tenax	-	-
P7/L1	A	GFF-T	GFF-U	-	-	$+Cl_2$	-	-	-	Tenax	Tenax	-	-
P9/L1	A	GFF-U	GFF-U	-	-	-	-	-	-	Tenax	Tenax	-	-
P9/L2	A	GFF-U	GFF-U	-	-	-	-	-	-	Tenax	Tenax	-	-
P11/L3	A	GFF-U	GFF-U	-	-	-	-	-	-	Tenax	Tenax	-	-
P13/L4	A	GFF-U	GFF-U	-	-	-	-	-	-	Tenax	Tenax	-	-

[a] See Table 45 for sampling protocol.

[b] See Fig. 21 for definition of configuration.

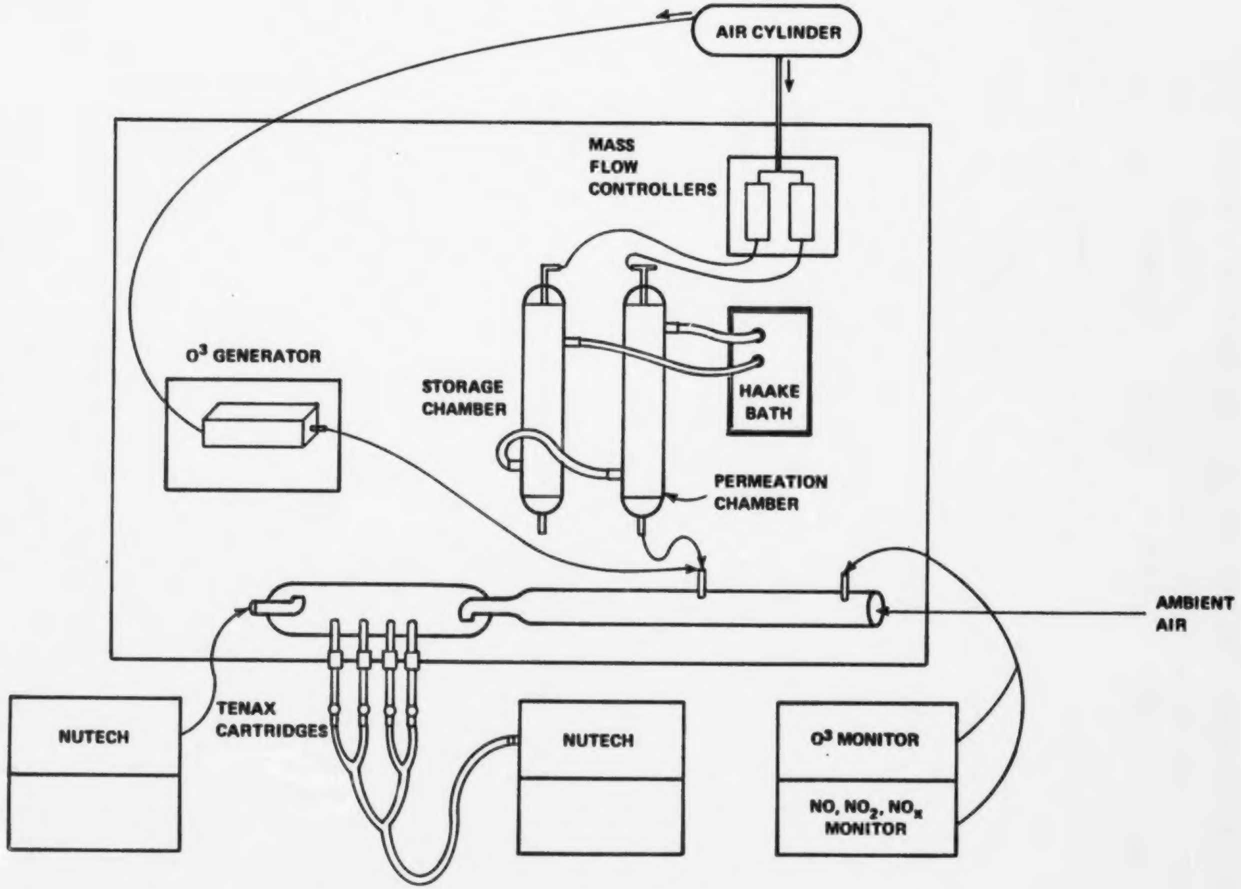

AIR CYLINDER
MASS FLOW CONTROLLERS
O^3 GENERATOR
STORAGE CHAMBER
HAAKE BATH
PERMEATION CHAMBER
AMBIENT AIR
TENAX CARTRIDGES
NUTECH
NUTECH
O^3 MONITOR
NO, NO_2, NO_x MONITOR

Figure 22. Schematic of instrumental devices used for in situ reaction studies of ambient air.

Table 8. EXPERIMENTAL DESIGN FOR IN SITU REACTION STUDIES

Experiment No.	U-GFF T_1	U-GFF T_2	T-GFF T_3	T-GFF T_4	Halogen
1	-	-	-	-	-
2	d_{10}-C	d_{10}-C	-	-	-
3	d_8-S	d_8-S	-	-	-
4	-	d_{10}-C	d_{10}-C	d_{10}-C	-
5	-	d_{10}-C	d_{10}-C	d_{10}-C	$+Cl_2$
6	-	d_{10}-C	d_{10}-C	d_{10}-C	$+Br_2$
7	-	d_8-S	d_8-C	d_8-C	-
8	-	d_8-S	d_8-C	d_8-C	$+Cl_2$
9	-	d_8-S	d_8-C	d_8-C	$+Br_2$

RESULTS AND DISCUSSION

Laboratory Studies

Analysis of Tenax cartridges that had been preloaded with d_{10}-cyclohexene and d_8-styrene and been exposed to ozone under laboratory conditions indicated the production of polar products. The polar products contained carbonyl moieties. Also a hydroxyl carbonyl compound was identified as a product from d_{10}-cyclohexene. In parallel experiments when the particulate filter proceding the Tenax GC cartridge was impregnated with sodium thiosulfate, the production of polar products was inhibited.

Field Studies

Baton Rouge, LA--

Three different atmospheric conditions were selected for field *in situ* reaction studies in Baton Rouge. The first was conducted during a period of time representing the highest level of ozone, the second during a high level of NO_x and auto exhaust, and finally the third during low levels of ozone (night). Ozone and NO_x levels were also measured during this phase of the study. The results of the ozone levels are presented in Table 9.

In each of the samples collected, the halogenated hydrocarbons were characterized and these results are summarized in Table 10. T_2-Samples (designation in the code) in all cases represent the adsorbent cartridge which was in line with a permeation tube containing either molecular halogen or dimethylamine-d_6. It is readily apparent that a number of chlorinated and brominated compounds were detected at trace levels which were not present in the corresponding controls. Also indicated in the table are the results for the *in situ* nitrosation reaction study (DMA-d_6). Trace levels of d_6-dimethylnitrosamine were tentatively detected.

The levels of halogenated hydrocarbons in the ambient air samples were estimated and these results are given in Tables 11-20. Table 11 presents the results obtained for ambient air and was compared with air sparged with chlorine. The compounds unaffected by the presence of chlorine are given in the upper portion of the table, whereas increased levels appeared for other compounds. Table 12 presents the similar experimental design; however, a permeation tube containing molecular bromine was used in the T_2 glass chamber instead of molecular chlorine. In this case methyl bromide, ethylene dibromide, bromoform and dibromocyclohexane were quantified.

Table 13 gives the results for dimethylamine-d_6 spiked in the ambient air. A trace quantity of dimethylnitrosamine-d_6 was detected.

The sparging of ambient air with molecular chlorine was repeated during a second sampling period which represented a period of high auto exhaust levels. Again chlorinated cyclohexanes were formed. In addition, a chlorophenol isomer was detected (Table 14).

Tables 19 and 20 list the estimated levels of halogenated compounds for ambient air with and without molecular chlorine and bromine added. In this

Table 9. OZONE CONCENTRATIONS IN BATON ROUGE, LA[a]

Hour	December, 1978		
	5th	6th	7th
1	0.001	0.000	0.000
2	0.000	0.00	0.000
3	0.000	0.000	0.000
4	0.000	0.000	0.000
5	0.000	0.000	0.000
6	0.000	0.000	0.000
7	0.000	0.000	0.000
8	0.000	0.000	0.000
9	0.000	0.000	0.000
10	0.001	0.002	0.002
11	0.010	0.014	0.004
12	0.026	*	0.010
13	0.029	*	0.005
14	0.022	0.047	0.008
15	0.022	0.041	0.005
16	0.024	0.043	0.003
17	0.017	0.033	0.000
18	0.000	0.019	0.000
19	0.000	0.017	0.000
20	0.000	0.019	0.000
21	0.000	0.018	0.000
22	0.000	0.010	0.000
23	0.000	0.004	0.000
24	0.000	0.001	0.000

[a] Data supplied by the Louisiana Air Control Commission from their L.S.U. Station.

*Performed calibration.

Table 10. SUMMARY OF THE DETECTION OF HALOGENATED COMPOUNDS AND NITROSAMINE IN AMBIENT AIR SPIKED WITH MOLECULAR HALOGENS AND DIMETHYLAMINE-D_6 IN BATON ROUGE, LA

Compound	Sample code										
	P1/L5A-1/T_1 (-)	P1/L5A-1/T_2 (+Br_2)	P1/L5A-2/T_1 (-)	P1/L5A-2/T_2 (+Cl_2)	P1/L5B-1/T_2 (+DMA-d_6)	P2/L5A-1/T_2 (+Br_2)	P2/L5B/T_2 (+Cl_2)	P2/L5C/T_2 (DMA-d_6)	P3/L5A/T_2 (+Br_2)	P3/L5B/T_2 (+Cl_2)	P3/L5C/T_2 (+DMA-d_6)
Methyl chloride	+	+	+	+	-	-	+	-	+	-	-
Methylene chloride	+	+	+	+	+	+	+	+	+	+	+
Chloroform	+	+	+	+	+	+	+	+	+	+	-
Carbon tetrachloride	-	+	+	+	+	+	+	-	+	+	+
1,2-Dichloroethane	+	+	+	+	+	+	+	+	+	+	+
1,1,1-Trichloroethane	+	+	+	+	+	+	+	+	+	+	+
Trichloroethylene	+	+	+	+	+	+	+	+	+	+	+
Tetrachloroethylene	+	+	+	+	+	+	+	+	+	+	+
1,2-Dichloropropane	-	-	-	-	+	-	-	-	-	-	-
Chlorocyclohexane isomer	-	-	-	+	-	-	+	-	-	+	-
Dichlorocyclohexane isomer	-	-	-	+	-	-	+	-	-	+	-
" "	-	-	-	+	-	-	+	-	-	-	-
Trichlorocyclohexane isomer	-	-	-	+	-	-	+	-	-	+	-
" "	-	-	-	+	-	-	+	-	-	+	-
" "	-	-	-	+	-	-	+	-	-	+	-
" "	-	-	-	-	-	-	-	-	-	+	-
Methyl bromide	-	+	-	-	-	+	-	-	+	-	-
Ethylene dibromide	-	+	-	-	-	+	-	-	-	-	-
Bromoform	-	+	-	+	-	+	+	-	+	+	-
Dibromocyclohexane isomer	-	+	-	-	-	+	-	-	-	-	-
Chlorobenzene	+	+	+	+	+	+	+	+	+	+	-
o-m-p-Dichlorobenzene(s)	+	+	+	+	+	+	+	-	-	+	+
Chlorophenol isomer	-	-	-	-	-	-	+	-	-	-	-
Dimethylnitrosamine-d_6 (tent.)	-	-	-	-	+	-	-	+	-	-	+

Table 11. ESTIMATION OF LEVELS OF HALOGENATED HYDROCARBONS IN SITU REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT CHLORINE ADDED

Chemical	$-Cl_2$[a]	$+Cl_2$[b]
	GFF-U	GFF-U
Ethylene dibromide	1,825[c]	1,547
1,1,1-Trichloroethane	164	171
Carbon tetrachloride	563	443
Trichloroethylene	55	79
Tetrachloroethylene	389	278
Benzene	989	1,135
Chloroform	725	1,099
Chlorobenzene	21	153
Dichlorobenzenes (2)	32	194
Dichlorohexanes (2)	ND	1,834
Trichlorohexanes (3)	ND	3,355
Chlorocyclohexane	ND	651

[a] $P1/L5A-2/T_1$.

[b] $P1/L5A-2/T_2$.

[c] Values are in ng, ND = not detected.

Table 12. ESTIMATION OF LEVELS OF HALOGENATED HYDROCARBONS *IN SITU* REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT BROMINE ADDED

Chemical	$-Br_2$[a] GFF-U	$+Br_2$[b] GFF-U
Chloroform	606[c]	642
Ethylene dichloride	1,794	1,427
1,1,1-Trichloroethane	173	246
Carbon tetrachloride	ND	ND
Tetrachloroethylene	371	304
Chlorobenzene	18	18
Benzene	669	916
Methyl bromide	ND	61
Ethylene dibromide	ND	28
Bromoform	ND	3,510
Dibromocyclohexane	ND	1,332

[a] $P1/L5A-1/T_1$.

[b] $P1/L5A-1/T_2$.

[c] Values are in ng, ND = not detected.

Table 13. ESTIMATION OF LEVELS FOR SELECTED ORGANICS IN SITU REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT DIMETHYLAMINE-D_6 ADDED

Chemical	-DMA-d_6[a]	+DMA-d_6[b]
	GFF-U	GFF-U
Chloroform	515[c]	338
1,2-Dichloroethane	1,557	945
1,1,1-Trichloroethane	224	112
Benzene	961	659
Carbon tetrachloride	273	195
1,2-Dichloropropane	24	19
Trichloroethylene	107	112
Dimethylnitrosamine-d_6	-	5
Chlorobenzene	22	18
Dichlorobenzene isomer	18	17

[a] P1/L5B/T_1.

[b] P1/L5B/T_2.

[c] Values in ng/cartridge, - = not detected.

Table 14. ESTIMATION OF LEVELS OF SELECTED ORGANICS *IN SITU* REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT CHLORINE ADDED

Chemical	$-Cl_2$[a]	$+Cl_2$[b]
	GFF-U	GFF-U
Chloroform	45[c]	109
Ethylene dichloride	7	70
1,1,1-Trichloroethane	624	40
Benzene	1,127	1,161
Carbon tetrachloride	47	38
Trichloroethylene	60	55
Tetrachloroethylene	59	39
Ethylene dibromide	17	126
Chlorobenzene	1	150
Bromoform	-	74
Chlorocyclohexane	19	172
Chlorophenol isomer	-	24
m-*p*-Dichlorobenzene	10	28
o-Dichlorobenzene	5	45
Dichlorocyclohexane isomer	15	921
Dichlorocyclohexane isomer	7	220
Trichlorocyclohexane isomer	-	245
Trichlorocyclohexane isomer	-	386
Trichlorocyclohexane isomer	-	789

[a] $P2/L5B/T_1$.

[b] $P2/L5B/T_2$.

[c] - = not detected, values in ng/cartridge.

Table 15. ESTIMATION OF LEVELS OF SELECTED ORGANICS *IN SITU* REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT DIMETHYLAMINE-D_6 ADDED

Chemical	-DMA-d_6[a]	+DMA-d_6[b]
	GFF-U	GFF-U
Chloroform	64[c]	37
Ethylene dichloride	84	76
1,1,1-Trichloroethane	145	105
Benzene	1,191	930
Trichloroethylene	112	57
Tetrachloroethylene	62	56
Dimethylnitrosamine-d_6	-	10
Chlorobenzene	15	5

[a] P2/L5C/T_1.

[b] P2/L5C/T_2.

[c] Values in ng/cartridge, - = not detected.

Table 16. ESTIMATION OF LEVELS OF SELECTED ORGANICS IN SITU REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT CHLORINE ADDED

Chemical	$-Cl_2$[a]	$+Cl_2$[b]
	GFF-U	GFF-U
Chloroform	ND[c]	284
1,2-Dichloroethane	ND	86
1,1,1-Trichloroethane	ND	145
Benzene	ND	1,538
Carbon tetrachloride	ND	137
Trichloroethylene	ND	183
Chlorocyclohexene isomer	ND	18
Tetrachloroethylene	65	169
Chlorobenzene	4	115
Chlorocyclohexane isomer	-	242
Dichlorobenzene isomer	14	33
Dichlorobenzene isomer	3	46
Dichlorocyclohexane isomer	-	1,587
Dichlorocyclohexane isomer	-	71
Trichlorocyclohexane isomer	-	395
Trichlorocyclohexane isomer	-	454
Trichlorocyclohexane isomer	-	655

[a] $P3/L5B/T_1$.

[b] $P3/L5B/T_2$.

[c] ND = not determined, - = not detected, values in ng/cartridge.

Table 17. ESTIMATION OF LEVELS OF SELECTED ORGANICS IN SITU REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT BROMINE ADDED

Chemical	-Br_2[a]	+Br_2[b]
	GFF-U	GFF-U
Chloroform	64[c]	95
1,2-Dichloroethane	75	76
1,1,1-Trichloroethane	204	197
Benzene	1,354	144
Carbon tetrachloride	130	117
Trichloroethylene	9	129
Tetrachloroethylene	73	147
Chlorobenzene	4	18
Bromoform	-	T

[a] P3/L5A/T_1.

[b] P3/L5A/T_2.

[c] - = not detected, values in ng/cartridge.

Table 18. ESTIMATION OF LEVELS OF SELECTED ORGANICS *IN SITU* REACTION STUDIES: AMBIENT AIR WITH AND WITHOUT DIMETHYLAMINE-D_6 ADDED

Chemical	-DMA-d_6[a]	+DMA-d_6[b]
	GFF-U	GFF-U
1,2-Dichloroethane	ND[c]	52
1,1,1-Trichloroethane	ND	99
Benzene	ND	848
Carbon tetrachloride	ND	91
Trichloroethylene	ND	49
Tetrachloroethylene	ND	45
Dimethylnitrosamine-d_6	-	10
Dichlorobenzene isomer	ND	12
Dichlorobenzene isomer	ND	5

[a] P3/L5C/T_1.

[b] P3/L5C/T_2.

[c] Values in ng/cartridge, - = not detected, ND = not determined.

Table 19. ESTIMATION OF LEVELS OF HALOGENATED COMPOUNDS EFFECT OF OZONE ON IN SITU REACTIONS: AMBIENT AIR WITH AND WITHOUT CHLORINE ADDED

Chemical	$-Cl_2$[a]	$+Cl_2$[b]	$+Cl_2$[c]	Cl_2[d]
	O_3 = 27 ppb	O_3 = 27	O_3 = 20	O_3 = 0
Chlorobenzene	21[e]	153	150	115
Dichlorobenzenes (2)	32	194	73	79
Dichlorohexanes (2)	ND	1,834	1,141	1,656
Trichlorohexanes (3)	ND	3,355	1,420	1,504
Chlorocyclohexane	ND	651	172	242

[a] P1/L5A-2/T_1.

[b] P1/L5A-2/T_2.

[c] P2/L5B/T_1.

[d] P3/L5B/T_2.

[e] Values in ng/cartridge.

Table 20. ESTIMATION OF LEVELS OF HALOGENATED COMPOUNDS EFFECT OF OZONE ON *IN SITU* REACTIONS: AMBIENT AIR WITH AND WITHOUT BROMINE ADDED

Chemical	$-Br_2$[a]	$+Br_2$[b]	$+Br_2$[c]	$+Br_2$[d]
	O_3 = 27 ppb	O_3 = 27	O_3 = 20	O_3 = 0
Methyl bromide	ND	61[a]	38	ND
Ethylene dibromide	ND	28	28	ND
Bromoform	ND	3,510	1,404	T
Dibromocyclohexane	ND	1,332	882	ND

[a] $P1/L5A-1/T_1$.

[b] $P1/L5A-1/T_2$.

[c] $P2/L5A-1/T_1$.

[d] $P2/L5B/T_2$.

[e] Values are in ng/cartridge.

case the three sampling periods are compared to contrast the levels of halogenated compounds that were formed under varying levels of ozone. When bromine was added to ambient air, it appears that ozone facilitated the bromination of organics, since at an ozone concentration of zero, the brominated organics disappeared to only a trace quantity.

Lake Charles, LA--

Table 21 presents the quantification of 22 selected organics. In Tables 22-27, sampling configurations A and B (Fig. 21) were compared for cases in which the ambient air was either spiked with molecular chlorine or bromine. These results indicate that considerably less chlorination of endogenous material occurred in contrast to the results obtained in Baton Rouge, LA.

Houston, TX--

In this experiment, the Tenax sampling cartridges were loaded with a discrete zone of d_{10}-cyclohexene (Table 28) or d_8-styrene (Table 29). The spiked cartridges were then taken to the field for use in sampling (configuration B, Fig. 21). Tables 29-32 present the vapor-phase halogenated and other selected organics which were identified in the ambient air from Houston. Quantitative analysis of these cartridges yielded the results shown in Figures 23 and 24 (also Tables 33 and 34).

Tables 35 and 36 summarize the results for the d_{10}-cyclohexene and d_8-styrene studies for the various configurational arrangements in sampling and the use of untreated and treated glass fiber filters with sodium thiosulfate.

Raleigh, NC--

Table 37 presents the sampling protocol for in situ reactions utilizing deuterated compounds sparged into the air sampling stream.

Tables 38-41 list the levels of deuterated compounds formed from d_{10}-cyclohexene or d_8-styrene and molecular chlorine or bromine, respectively.

Table 21. QUANTIFICATION OF IN SITU REACTIONS IN AMBIENT AIR OF LAKE CHARLES, LA[a]

Chemical	Sample code				
	P1/L1-A/T_1 (+Cl_2)	P1/L1-A/T_2 (-)	P1/L1-A/T_3 (+Br_2)	P1/L1-A/T_4 (-)	P1/L1-B/T_4 (+Br_2)
Benzene	277	208	208	225	ND
Vinylidene chloride	131	ND	ND	ND	ND
Chloroform	90	129	56	115	ND
Carbon tetrachloride	43	48	34	42	ND
1,2-Dichloroethane	117	117	82	98	ND
1,1,1-Trichloroethane	106	ND	83	ND	ND
Trichloroethylene	76	55	63	62	ND
Tetrachloroethylene	56	56	57	70	ND
Dichlorobenzene isomer	8	8	6	6	ND
Dichlorobenzene isomer	ND	T	ND	T	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND
1,1,2-Trichloroethane	ND	ND	ND	ND	ND
1,1,1,2-Tetrachloroethane	ND	ND	ND	ND	ND
Chlorobenzene	ND	ND	ND	ND	ND
1,1,2,2-Tetrachloroethane	130	ND	81	ND	ND
1,3,5-Trichlorobenzene	ND	ND	ND	ND	ND
Pentachloroethane	ND	ND	ND	ND	ND
Pentachlorobromoethane	ND	ND	ND	ND	ND

(continued)

Table 21 (cont'd.)

Chemical	Sample code				
	P1/L1-A/T_1 (+Cl_2)	P1/L1-A/T_2 (-Cl_2)	P1/L1-A/T_3 (+Br_2)	P1/L1-A/T_4 (-Br_2)	P1/L1-B/T_4 (+Br_2)
Pentachlorobutadiene	ND	ND	ND	ND	ND
Hexachlorobutadiene	ND	ND	ND	ND	ND
Bromoform	ND	ND	582	ND	ND
Dibromocyclohexane isomer	ND	ND	338	ND	538
Chloromethylbutene isomer	T	ND	ND	ND	ND

[a] See Table 6 for experimental design.

Table 22. QUANTIFICATION OF IN SITU REACTIONS IN AMBIENT AIR OF LAKE CHARLES, LA[a]

Chemical	Sample Code					
	P3/L1-A/T_1 (-)	P3/L1-A/T_2 (+Br_2)	P3/L1-B1/T_1 (-)	P3/L1-B1/T_2 (+Cl_2)	P3/L1-B2/T_1 (-)	P3/L1-B2/T_2 (+Br_2)
Benzene	390	442	503	257	390	341
Vinylidene chloride	T	T	106	ND	T	113
Chloroform	163	79	118	107	163	38
Carbon tetrachloride	39	36	46	46	39	34
1,2-Dichloroethane	73	76	81	58	73	56
1,1,1-Trichloroethane	128	83	60	30	128	26
Trichloroethylene	65	33	43	20	65	T
Tetrachloroethylene	39	38	34	24	39	22
Dichlorobenzene isomer	5	6	13	6	5	T
Dichlorobenzene isomer	ND	T	T	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND	ND
1,1,2-Trichloroethane	ND	33	49	ND	ND	ND
1,1,1,2-Tetrachloroethane	ND	ND	ND	ND	ND	ND
Chlorobenzene	43	23	21	7	ND	ND
1,1,2,2-Tetrachloroethane	ND	88	ND	ND	43	219
1,3,5-Trichlorobenzene	ND	ND	ND	ND	ND	ND
Pentachloroethane	ND	ND	ND	ND	ND	ND
Hexachlorobutadiene	ND	ND	ND	ND	ND	ND
Bromoform	ND	227	ND	ND	ND	ND
Dibromocyclohexane isomer	ND	95	ND	ND	ND	74
Chloromethylbutene isomer	115	ND	ND	ND	ND	40
			ND	531	115	ND

[a] See Table 6 for experimental design.

Table 23. QUANTIFICATION OF IN SITU REACTIONS IN AMBIENT AIR OF LAKE CHARLES, LA[a]

Chemical	Sample Code				
	P4/L1-A1/T_1 (-)	P4/L1-A1/T_2 (+Cl_2)	P4/L1-A2/T_1 (-)	P4/L1-A2/T_3 (+Br_2)	P4/L1-B/T_2 (+Br_2)
Benzene	84	289	237	280	286
Vinylidene chloride	ND	4,220	3,448	1,880	3,808
Chloroform	62	68	51	600	84
Carbon tetrachloride	27	36	31	T	39
1,2-Dichloroethane	104	67	62	19	89
1,1,1-Trichloroethane	15	29	37	75	83
Trichloroethylene	121	74	55	20	67
Tetrachloroethylene	50	42	26	55	52
Dichlorobenzene isomer	9	12	T	T	ND
Dichlorobenzene isomer	ND	T	ND	ND	ND
Dichlorobenzene isomer	ND	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND
1,1,2-Trichloroethane	ND	ND	ND	ND	ND
1,1,1,2-Tetrachloroethane	ND	ND	ND	ND	ND
Chlorobenzene	50	6	ND	ND	4
1,1,2,2-Tetrachloroethane	ND	88	116	16	17
1,3,5-Trichlorobenzene	ND	ND	ND	ND	ND
Pentachloroethane	ND	ND	ND	ND	ND

(continued)

Table 23 (cont'd.)

Chemical	Sample code				
	P4/L1-A1/T_1 (-)	P4/L1-A1/T_2 (+Cl_2)	P4/L1-A2/T_1 (-)	P4/L1-A2/T_3 (+Br_2)	P4/L1-B/T_2 (+Br_2)
Pentachlorobromoethane	ND	ND	ND	ND	ND
Pentachlorobutadiene	ND	ND	ND	ND	ND
Hexachlorobutadiene	ND	ND	ND	ND	ND
Bromoform	ND	ND	T	314	ND
Dibromocyclohexane isomer	ND	ND	ND	32	166
Chloromethylbutene isomer	ND	145	ND	72	ND

[a] See Table 6 for experimental design.

Table 24. QUANTIFICATION OF IN SITU REACTIONS IN AMBIENT AIR IN LAKE CHARLES, LA[a]

Chemical	Sample code				
	P5/L1-B1/T_1 (-)	P5/L1-B1/T_2 (+Cl_2)	P5/L1-B2/T_2 (+Br_2)	P5/L1-A/T_1[b] (-)	P5/L1-A/T_3 (+Br_2)
Benzene	147	156	ND	113	199
Vinylidene chloride	201	ND	329	ND	226
Chloroform	293	642	391	354	698
Carbon tetrachloride	49	51	62	44	48
1,2-Dichloroethane	596	490	160	490	756
1,1,1-Trichloroethane	83	136	128	106	128
Trichloroethylene	78	102	121	78	119
Tetrachloroethylene	464	447	514	388	379
Dichlorobenzene isomer	5	9	5	T	4
Dichlorobenzene isomer	ND	T	ND	T	T
1,2-Dichloroethylene isomer	87	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND	ND
1,1,2-Trichloroethane	75	36	ND	50	35
1,1,1,2-Tetrachloroethane	ND	ND	ND	ND	ND
Chlorobenzene	ND	ND	ND	ND	ND
1,1,2,2-Tetrachloroethane	ND	ND	ND	ND	ND
1,3,5-Trichlorobenzene	ND	ND	ND	ND	ND
Pentachloroethane	ND	ND	ND	ND	ND

(continued)

Table 24 (cont'd.)

Chemical	Sample code				
	P5/L1-B1/T_1 (-)	P5/L1-B1/T_2 (+Cl_2)	P5/L1-B2/T_2 (+Br_2)	P5/L1-A/T_1[b] (-)	P5/L1-A/T_3 (+Br_2)
Pentachlorobutadiene	ND	ND	ND	ND	ND
Hexachlorobutadiene	T	69	T	ND	T
Bromoform	ND	ND	122	ND	196
Dibromocyclohexane isomer	ND	ND	ND	ND	104
Chloromethylbutene isomer	ND	ND	216	ND	ND

[a] See Table 6 for experimental design.

[b] P5/L1-A/T_1 = P5/L1-B2/T_1 (control).

Table 25. QUANTIFICATION OF *IN SITU* REACTIONS IN AMBIENT AIR IN LAKE CHARLES, LA[a]

Chemical	Sample code			
	$P6/L1\text{-}B/T_1$ (-)	$P6/L1\text{-}B/T_2$ ($+Cl_2$)	$P8/L1\text{-}A/T_1$ (-)	$P8/L1\text{-}A/T_2$ ($+Cl_2$)
Benzene	6,369	457	376	436
Vinylidene chloride	ND	ND	ND	139
Chloroform	214	96	175	670
Carbon tetrachloride	32	41	256	4,393
1,2-Dichloroethane	1,639	1,416	426	426
1,1,1-Trichloroethane	76	76	56	106
Trichloroethylene	82	72	80	88
Tetrachloroethylene	70	83	55	65
Dichlorobenzene isomer	7	5	5	29
Dichlorobenzene isomer	T	T	ND	28
1,2-Dichloroethylene isomer	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND
1,1,2-Trichloroethane	ND	ND	ND	ND
1,1,1,2-Tetrachloroethane	ND	ND	ND	ND
Chlorobenzene	4	4	4	9
1,1,2,2-Tetrachloroethane	ND	ND	ND	ND
1,3,5-Trichlorobenzene	ND	ND	ND	T
Pentachloroethane	ND	ND	ND	ND

(continued)

Table 25 (cont'd.)

Chemical	Sample code			
	P6/L1-B/T_1 (-)	P6/L1-B/T_2 (+Cl_2)	P8/L1-A/T_1 (-)	P8/L1-A/T_2 (+Cl_2)
Pentachlorobromoethane	ND	ND	ND	ND
Pentachlorobutadiene	ND	ND	ND	ND
Hexachlorobutadiene	ND	ND	ND	ND
Bromoform	ND	ND	ND	ND
Dibromocyclohexane isomer	ND	ND	ND	ND
Chloromethylbutene isomer	ND	ND	ND	ND

[a] See Table 6 for experimental design.

Table 26. QUANTIFICATION OF IN SITU REACTIONS IN AMBIENT AIR IN LAKE CHARLES, LA[a]

Chemical	Sample code			
	P9/L1-A/T_1 (-)	P9/L1-A/T_2 (+Cl_2)	P10/L1-B/T_1 (-)	P10/L1-B/T_2 (+Cl_2)
Benzene	387	439	324	384
Vinylidene chloride	ND	ND	ND	ND
Chloroform	152	349	366	636
Carbon tetrachloride	188	144	65	62
1,2-Dichloroethane	255	255	64	69
1,1,1-Trichloroethane	69	67	79	121
Trichloroethylene	47	76	86	90
Tetrachloroethylene	66	59	67	35
Dichlorobenzene isomer	6	T	T	4
Dichlorobenzene isomer	T	T	ND	T
1,2-Dichloroethylene isomer	ND	ND	ND	ND
1,2-Dichloroethylene isomer	ND	ND	ND	ND
1,1,2-Trichloroethane	ND	ND	ND	ND
1,1,1,2-Tetrachloroethane	ND	ND	ND	ND
Chlorobenzene	ND	11	14	19
1,1,2,2-Tetrachloroethane	ND	ND	ND	ND
1,3,5-Trichlorobenzene	ND	ND	ND	ND
Pentachloroethane	ND	ND	ND	ND

(continued)

Table 26 (cont'd.)

Chemical	Sample code			
	$P9/L1\text{-}A/T_1$ (-)	$P9/L1\text{-}A/T_2$ ($+Cl_2$)	$P10/L1\text{-}B/T_1$ (-)	$P10/L1\text{-}B/T_2$ ($+Cl_2$)
Pentachlorobromoethane	ND	ND	ND	ND
Pentachlorobutadiene	ND	ND	ND	ND
Hexachlorobutadiene	ND	ND	ND	ND
Bromoform	ND	ND	ND	ND
Dibromocyclohexane isomer	ND	ND	ND	ND
Chloromethylbutene isomer	ND	ND	69	ND

[a] See Table 6 for experimental design.

Table 27. EXPERIMENTAL DESIGN FOR SAMPLING WITH TENAX CARTRIDGES LOADED WITH CYCLOHEXENE-D_{10}

Sample code	Cartridge no.	Cyclohexene-d_{10}[a]	$Na_2S_2O_3$[b]	Halogen (μg)[c]	O_3[d] (ppb)
P1/L1	T1	-	-	- (0)	35
	T2	1 μg	-	- (0)	35
	T3	1 μg	1%	- (0)	35
	T4	1 μg	10%	- (0)	35
P2/L1	T1	-	-	+ (11.3)	37
	T2	1 μg	-	+ (11.3)	37
	T3	1 μg	1%	+ (11.3)	37
	T4	1 μg	10%	+ (11.3)	37
P3/L1	T1	-	-	+ (11.4)	28
	T2	1 μg	-	+ (11.4)	28
	T3	1 μg	1%	+ (11.4)	28
	T4	1 μg	10%	+ (11.4)	28

[a] Cyclohexene-d_{10} (nominal level) was loaded onto Tenax GC cartridge prior to sampling.

[b] Glass fiber filter was impregnated with aqueous solution of $Na_2S_2O_3$.

[c] Cl_2 permeation rate was 1.24×10^{6} g/min and added to ambient air to give final concentration of 39 ppb, thus 11.3 μg passed through each cartridge. Br_2 permeation rate was 7.65×10^{7} g/min and added to ambient air to give final concentration of 17.5 ppb, thus 11.4 μg passed through each cartridge.

[d] O_3 was measured in ambient air sampled.

Table 28. EXPERIMENTAL DESIGN FOR SAMPLING WITH TENAX CARTRIDGES LOADED WITH STYRENE-D_8

Sample code	Cartridge no.	Styrene-d_8[a]	$Na_2S_2O_3$[b]	Halogen (µg)[c]	O_3[d] (ppb)
P1/L1	T1	-	-	- (0)	26
	T2	1 µg	-	- (0)	26
	T3	1 µg	1%	- (0)	26
	T4	1 µg	10%	- (0)	26
P2/L1	T1	-	-	Cl_2 (11.1)	26
	T2	1 µg	-	Cl_2 (11.1)	26
	T3	1 µg	1%	Cl_2 (11.1)	26
	T4	1 µg	10%	Cl_2 (11.1)	26
P3/L1	T1	-	-	Br_2 (11.7)	28
	T2	1 µg	-	Br_2 (11.7)	28
	T3	1 µg	1%	Br_2 (11.7)	28
	T4	1 µg	10%	Br_2 (11.7)	28

[a] Styrene-d_8 (approximate quantity) was loaded with Tenax GC cartridges prior to sampling.

[b] Glass fiber filter was impregnated with aqueous solution of $Na_2S_2O_3$.

[c] Cl_2 permeation rate was 1.24 x 10^{-6} g/min, 38 ppb in ambient air, and 11.1 µg through each cartridge. Br_2 permeation rate was 7.65 x 10^{-7} g/min and added to ambient air, 1 ppb in air, 11.7 µg through each cartridge.

[d] O_3 was measured in ambient air.

Table 29. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM HOUSTON, TX (P1/L1-A/T_1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2	18	96	1,2-dibromoethane (traces)
2	46	chloromethane (traces) (tent.)	19	101	tetrachloroethylene
3	49	bromomethane (traces)	20	104	C_7D_{12} or $C_6D_{10}O$ isomer
4	54	methylene chloride	21	108	C_7D_{12} isomer
5	63	hexafluorobenzene (eB)	22	113	unknown deuterium compound
6	64	chloroform	23	114	bromoform
7	67	perfluorotoluene (eB)	24	118	bicycloheptene-d_{10} or C_7D_{10} isomer
8	68	1,2-dichloroethane	25	122	2,3-dichloropropanol-1 (tent.)
9	69	1,1,1-trichloroethane	26	140	2-chloro-d_{10}-cyclohexanol
10	71	d_6-benzene	27	144	dichlorobenzene isomer (trace)
11	72	benzene	28	148	dichloro-d_{10}-cyclohexane isomer
12	72	carbon tetrachloride	29	162	dichloro-d_{10}-cyclohexane isomer (tent.)
13	73	d_8-cyclohexadiene	30	164	dusterium compound unknown
14	76	d_{10}-cyclohexene	31	177	hexachlorobutadiene
15	79	trichloroethylene + bromodichloromethane			
16	92	toluene			
17	95	dibromochloromethane			

[a] See Tables 45 and 7 for protocol and experimental design.

Table 30. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM HOUSTON, TX (P1/L1-A/T3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2	54	methylene chloride
3	62	hexafluorobenzene (eI)
4	63	chloroform (traces)
5	66	perfluorotoluene (eI)
6	67	1,2-dichloroethane
7	68	1,1,1-trichloroethane
8	70	d_6-benzene
9	71	benzene
10	71	carbon tetrachloride
11	72	d_8-cyclohexadiene
12	74	d_{10}-cyclohexene
13	78	trichloroethylene
14	91	toluene
15	95	1,2-dibromoethane
16	100	tetrachloroethylene
17	107	C_7D_{12} isomer
18	112	bromoform
19	118	C_7D_{10} or unknown
20	123	bromobenzene
21	138	dichlorobenzene isomer (trace)
22	141	dichlorobenzene isomer (trace)
23	151	pentachlorobromoethane (tent.) (traces)
24	160	dichloro-d_{10}-cyclohexane isomer (tent.)
25	174	dibromo-d_{10}-cyclohexane isomer
26	176	dibromocyclohexane isomer

[a] See Tables 45 and 7 for sampling and experimental design.

Table 31. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM HOUSTON, TX (P3/L1-A/T_1)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2	48	bromomethane (traces)
3	54	methylene chloride
4	59	hexafluorobenzene (sS)
5	63	perfluorotoluene (sS)
6	63	1,2-dichloroethane
7	64	1,1,1-trichloroethane
8	69	carbon tetrachloride
9	71	d_{10}-cyclohexene
10	78	trichloroethylene
11	95	1,2-dibromoethane
12	99	tetrachloroethylene
13	106	chlorobenzene
14	112	bromoform
15	115	d_8-styrene
16	122	bromobenzene
17	137	dichlorobenzene
18	141	dichlorobenzene isomer (trace)
19	168	dibromobenzene isomer (trace)
20	174	dibromo-d_{10}-cyclohexane isomer
21	175	dibromocyclohexane isomer

[a] See Tables 45 and 7 for sampling and experimental protocols.

Table 32. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM HOUSTON, TX (P4/L1-A/T_3)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2	54	methylene chloride
3	62	hexafluorobenzene (eS)
4	63	chloroform
5	66	perfluorotoluene (eS)
6	67	1,2-dichloroethane
7	68	1,1,1-trichloroethane
8	71	benzene
9	72	carbon tetrachloride (traces)
10	77	trichloroethylene (traces)
11	91	toluene
12	100	tetrachloroethylene
13	107	chlorobenzene
14	110	d_{10}-ethylbenzene
15	116	d_8-styrene
16	128	d_6-benzaldehyde
17	139	dichlorobenzene isomer (trace)
18	147	dichloro-d_{10}-cyclohexane isomer
19	149	d_7-chlorostyrene
20	156	d_7-chlorostyrene isomer
21	158	d_7-chlorostyrene isomer
22	180	d_8-styrene dichloride

[a] See Tables 45 and 7 for sampling and experimental protocols.

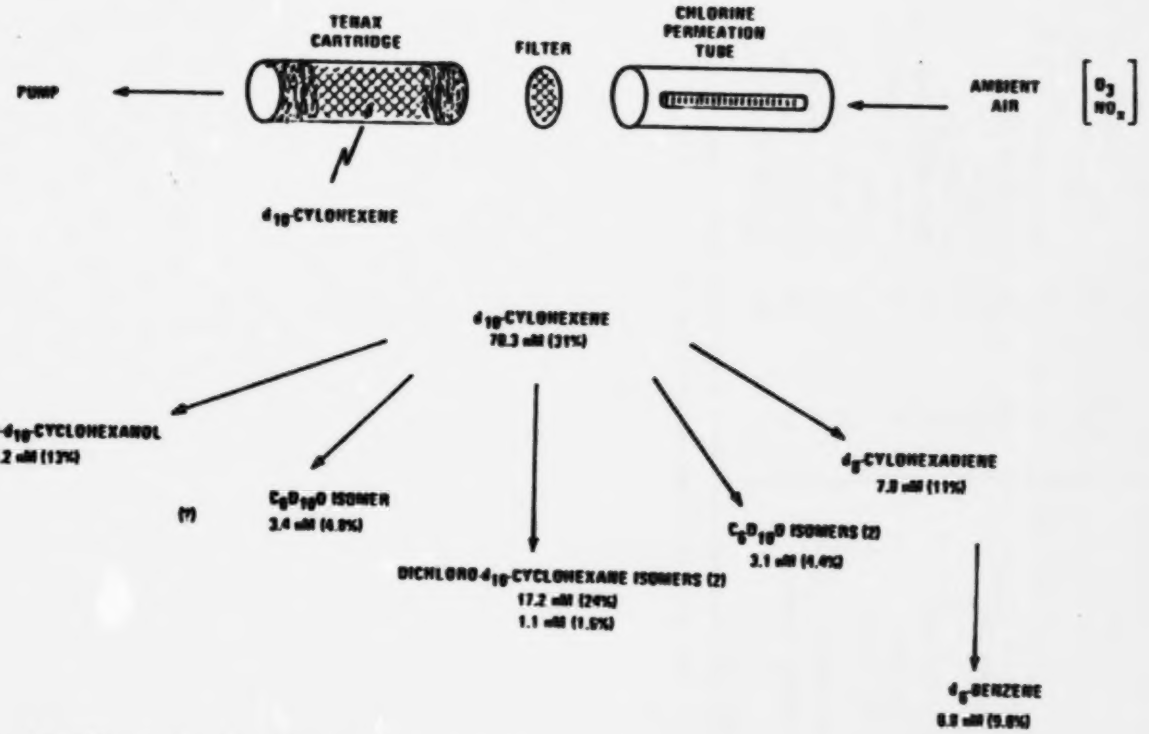

TENAX CARTRIDGE
FILTER
CHLORINE PERMEATION TUBE
PUMP
AMBIENT AIR
$\begin{bmatrix} O_3 \\ NO_x \end{bmatrix}$
d_{10}-CYLOHEXENE
d_{10}-CYLOHEXENE
70.3 mM (31%)
2-CHLORO-d_{10}-CYCLOHEXANOL
9.2 mM (13%)
(?)
$C_6D_{10}O$ ISOMER
3.4 mM (4.8%)
DICHLORO-d_{10}-CYCLOHEXANE ISOMERS (2)
17.2 mM (24%)
1.1 mM (1.6%)
$C_6D_{10}O$ ISOMERS (2)
3.1 mM (4.4%)
d_8-CYLOHEXADIENE
7.8 mM (11%)
d_6-BENZENE
6.8 mM (9.6%)

Figure 23. In situ reactions during ambient air sampling: d_{10}-cyclohexene.

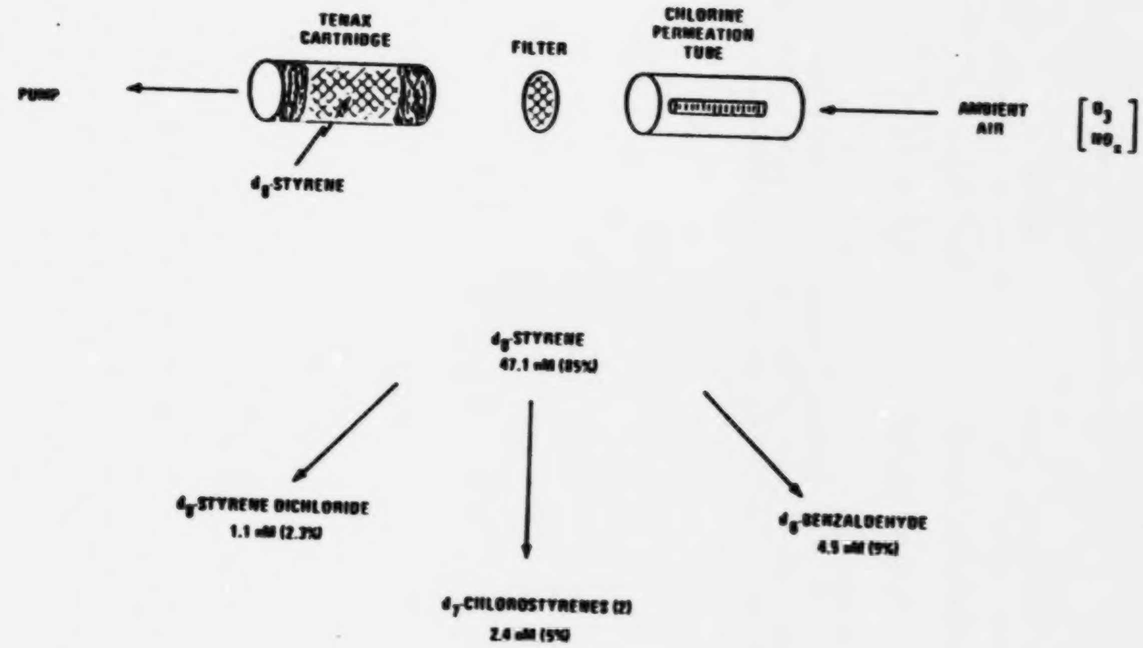

TENAX CARTRIDGE
FILTER
CHLORINE PERMEATION TUBE
PUMP
AMBIENT AIR
O_3
NO_x
d_8-STYRENE
d_8-STYRENE
47.1 nM (85%)
d_8-STYRENE DICHLORIDE
1.1 nM (2.3%)
d_7-CHLOROSTYRENES (2)
2.4 nM (5%)
d_8-BENZALDEHYDE
4.5 nM (9%)

Figure 24. In situ reactions during ambient air sampling: d_8-styrene.

Table 33. *IN SITU* REACTION YIELDS FROM D_{10}-CYCLOHEXENE AND MOLECULAR CHLORINE

Compound	$\frac{+Cl_2}{GFF\text{-}U}$[a]	$\frac{+Cl_2}{GFF\text{-}T}$
Dichloro-d_{10}-cyclohexane isomer	17.2 (24)	0
Dichloro-d_{10}-cyclohexane isomer	1.1 (1.6)	0
2-Chloro-d_{10}-cyclohexanol	9.2 (13)	0.5 (0.7)

[a] GFF-U = untreated glass fiber filter; GFF-T = glass fiber filter treated with 1% solution sodium thiosulfate; values are in nM with percent yield in parentheses.

Table 34. IN SITU REACTION YIELDS FROM D_8-STYRENE AND MOLECULAR CHLORINE

Compound	$-Cl_2$[a] GFF-U	$+Cl_2$ GFF-U	$+Cl_2$ GFF-T
d_7-Chlorostyrene isomer	0	0.25 (0.5)	0
d_7-Chlorostyrene isomer	0	2.04 (4.3)	0
d_8-Styrene dichloride	0	1.14 (2.4)	0

[a] -, + = without and with Cl_2 added to ambient air; GFF-U = untreated glass fiber filter; GFF-T = glass fiber filter impregnated with 1% solution sodium thiosulfate; values are in nM and percent yield given in parentheses.

Table 35. SUMMARY OF d_{10}-CYCLOHEXENE STUDY WITH AND WITHOUT MOLECULAR HALOGEN ADDED TO HOUSTON, TX AMBIENT AIR

Compound	No halogens				$+Cl_2$				$+Br_2$				Blank
	P1/L1/T1	P1/L1/T2	P1/L1/T3	P1/L1/T4	P2/L1/T1	P2/L1/T2	P2/L1/T3	P2/L1/T4	P3/L1/T1	P3/L1/T2	P3/L1/T3	P1/L1/T4	
Chloroform	ND	ND	ND	ND	2	13	-	T	ND	ND	ND	ND	
Carbon tetrachloride	ND	ND	ND	ND	T	10	T	T	ND	ND	ND	ND	
Chlorobenzene	ND	ND	ND	ND	14	25	12	10	ND	ND	ND	ND	
Dichlorobenzene isomer	ND	ND	ND	ND	-	11	-	T	ND	ND	ND	ND	
Dichlorobenzene isomer	ND	ND	ND	ND	-	14	-	-	ND	ND	ND	ND	
Methyl chloroform	ND	ND	ND	ND	T	16	T	T	ND	ND	ND	ND	
Trichloroethylene	ND	ND	ND	ND	T	14	T	T	ND	ND	ND	ND	
Tetrachloroethylene	ND	ND	ND	ND	T	16	16	T	ND	ND	ND	ND	
d_{10}-Cyclohexene	-	1,253	1,080	1,445	-	1,599	2,142	2,046	-	1,454	1,549	1,594	
d_8-Cyclohexadiene	-	6	11	16	-	100	29	30	-	20	23	27	
d_6-Benzene	-	11	10	18	-	158	32	52	-	21	25	30	
$C_6D_{10}O$ isomer	-	6	31	6	-	28	5	-	-	6	6	9	
$C_6D_{10}O$ isomer	-	150	4	18	-	36	18	-	-	9	25	33	
$C_6D_{10}O$ isomer	-	12	14	8	-	120	-	-	-	21	12	12	
Dichloro-d_{10}-cyclohexane isomers	-	-	-	-	-	1,080	2	23	-	-	-	-	
Dichlorocyclohexane isomer	-	-	-	-	-	-	-	-	-	-	-	-	
2-Chloro-d_{10}-Cyclohexanol	-	-	-	-	-	158	-	-	-	-	-	-	
2-Chlorohexanol	-	-	-	-	-	-	-	-	-	-	-	-	
2-Bromo-d_{10}-cyclohexanol	-	-	-	-	-	-	-	-	-	-	-	-	
Dibromo-d_{10}-cyclohexane isomers	-	-	-	-	-	-	-	-	-	515	568	568	
Dibromocyclohexane isomers	-	-	-	-	-	-	-	-	342	317	251	228	
Bromoform	-	-	-	-	-	-	-	-	319	426	194	97	
1,2-Dibromoethane	-	-	-	-	-	-	-	-	T	32	97	32	

Table 36. SUMMARY OF d_8-STYRENE STUDY WITH AND WITHOUT MOLECULAR HALOGEN ADDED TO HOUSTON, TX AMBIENT AIR

Compound	No halogen				$+Cl_2$				$+Br_2$				Blank
	P1/L1/T1	P1/L1/T2	P1/L1/T3	P1/L1/T4	P2/L1/T1	P2/L1/T2	P2/L1/T3	P2/L1/T4	P3/L1/T1	P3/L1/T2	P3/L1/T3	P3/L1/T4	
1,2-Dichloroethane	-	T	T	-	-	-	-	-	-	-	-	-	-
1,1,1-Trichloroethane	5	4	T	6	10	7	T	9	7	T	T	-	-
Carbon tetrachloride	5	T	T	T	13	7	T	8	9	T	9	8	-
Trichloroethylene	-	T	T	T	T	T	T	14	T	T	T	T	-
Tetrachloroethylene	-	T	T	T	7	6	10	11	12	10	T	7	-
Chlorobenzene	11	15	27	12	T	18	14	10	7	T	7	-	-
Dichlorobenzene isomer	T	T	T	-	T	T	T	T	T	T	T	-	-
Dichlorobenzene isomer	-	-	-	-	-	3	T	T	-	T	-	-	-
d_8-Styrene	-	757	789	1,168	-	1,432	1,291	1,392	-	1,300	1,400	1,490	1,540
d_6-Benzaldehyde	-	96	69	84	-	113	113	209	-	183	131	96	96
d_6-Acetophenone	-	-	-	-	-	-	T	T	-	-	-	-	-
d_6-Phenylacetylene	-	-	-	-	-	-	-	-	-	-	-	-	-
Chlorostyrene-d_7 isomer	-	-	-	-	-	-	-	-	-	-	-	-	-
Chlorostyrene-d_7 isomer	-	-	-	-	-	-	-	-	-	-	-	-	-
d_8-Styrene dichloride	-	-	-	-	-	-	-	-	-	-	-	-	-
Dibromobenzene	-	-	-	-	-	-	-	-	-	-	-	-	-
Dibromocyclohexane	-	-	-	-	-	-	-	-	228	216	224	244	-
Bromoform	-	-	-	-	-	-	-	-	692	266	29	34	-

Table 37. SAMPLING AND EXPERIMENTAL PROTOCOL FOR IN SITU REACTION STUDIES[a]

Sampling Period	U-GFF[b]	U-GFF	T-GFF[c]	T-GFF[d]	Halogen	O_3 ppb	NO ppb	Sample Volume (ℓ)	Remarks		
	T_1	T_2	T_3	T_4					Date	Temp.	Time
P01	-	-	-	-	-	-	-	0	-	-	
P02	d_{10}-C	d_{10}-C	-	-	-	-	-	0	-	-	
P03	d_8-S	d_8-S	-	-	-	-	-	0	-	-	
P1	-	d_{10}-C	d_{10}-C	d_{10}-C	-	36	0	98	8/30/79	91°F	15:07-16:07
P2	-	d_{10}-C	d_{10}-C	d_{10}-C	$+Cl_2$	37	0	99	8/30/79	92°F	16:22-17:22
P3	-	d_{10}-C	d_{10}-C	d_{10}-C	$+Br_2$	30	0	100	8/30/79	89°F	17:34-18:34
P4	-	d_8-S	d_8-C	d_8-C	-	26	0	98	9/6/79	90°F	14:00-15:00
P5	-	d_8-S	d_8-C	d_8-C	$+Cl_2$	24	0	99	9/6/79	90°F	15:10-16:10
P6	-	d_8-S	d_8-C	d_8-C	$+Br_2$	30	0	98	9/6/79	90°F	16:20-17:20

[a] Site was at Tryon Hills, Raleigh, NC.

[b] U-GFF = untreated glass fiber filter, d_{10}-C = cyclohexene-d_{10} and d_8-S = styrene-d_8.

[c] T-GFF = glass fiber filter with 1% sodium thiosulfate.

[d] T-GFF = glass fiber filter treated with 10% sodium thiosulfate.

Table 38. QUANTIFICATION OF IN SITU REACTIONS INVOLVING D_{10}-CYCLOHEXENE AND MOLECULAR CHLORINE[a]

Compound	Sample Code			
	P1/L1-A/T1	P1/L1-A/T2	P3/L1-A/T3	P3/L1-A/T4
d_6-Benzene	575	4	576	6
d_8-Cyclohexadiene	704	171	307	6
d_{10}-Cyclohexene	1,094	1,145	1,958	1,593
C_7D_{12} or $C_6D_{10}O$ isomer	335	ND	231	ND
C_7D_{12} isomer	245	14	150	ND
C_7D_{10} isomer	57	18	81	43
Dichloro-d_{10}-cyclohexane isomer	2,788	ND	342	ND
Dichloro-d_{10}-cyclohexane isomer	185	ND	ND	ND
2-Chloro-d_{10}-cyclohexanol	1,334	73	330	ND

[a] See Table 37 for experimental protocol, values in ng/cartridge.

Table 39. QUANTIFICATION OF IN SITU REACTIONS INVOLVING D_8-STYRENE AND MOLECULAR CHLORINE[a]

Compound	P4/L1-A/T3	P4/L1-A/T4	P6/L1-A/T1	P6/L1-A/T2
d_8-Styrene	4,180	3,526	4,080	3,395
d_6-Benzaldehyde	475	237	307	445
d_7-Chlorostyrene isomer	36	ND	ND	ND
d_7-Chlorostyrene isomer	298	ND	ND	ND
d_8-Styrene dichloride	209	ND	ND	ND

[a] See Table 37 for experimental protocol, values in ng/cartridge.

Table 40. QUANTIFICATION OF IN SITU REACTIONS INVOLVING D_{10}-CYCLOHEXENE AND MOLECULAR BROMINE[a]

Compound	P1/L1-A/T3	P1/L1-A/T4
d_6-Benzene	40	17
d_8-Cyclohexadiene	48	97
d_{10}-Cyclohexene	1,076	1,126
C_7D_{12} or $C_6D_{10}O$ isomer	13	11
C_7D_{12} isomer	19	14
C_7D_{10} isomer	44	21
Dibromo-d_{10}-cyclohexane isomer	6,258	1,442
Dibromocyclohexane isomer	1,033	ND

[a] See Table 37 for experimental protocol, values in ng/cartridge.

Table 41. QUANTIFICATION OF IN SITU REACTIONS INVOLVING D_8-STYRENE AND MOLECULAR BROMINE[a]

Compound	P3/L1-A/T1	P3/L1-A/T2
d_8-Styrene	756	646
d_6-Benzaldehyde	264	47

[a] See Table 37 for experimental protocol, values in ng/m^3.

SECTION 8

QUALITATIVE AND QUANTITATIVE ANALYSIS OF VAPOR-PHASE ORGANICS IN AMBIENT AIR

INTRODUCTION

During the evaluation of the basic GC/MS/computer system for the analysis of vapor-phase organics in ambient air, the improved methods were applied to the analysis of several industrial atmospheres for the presence of mutagenic and carcinogenic vapors. This section presents the results on the qualitative analysis of vapor-phase organics in air for several geographical areas.

In using a GC/MS/COMP system for the purpose of quantification of selected organic compounds in ambient air, it is important that instrument parameters be standardized in order to obtain reproducible and accurate data. In order to achieve reproducible and accurate quantitative data from a mass spectrometer, a number of criteria have been delineated which serve as guidelines to achieve this objective. These are:

(1) the selection of a standard compound which represents the $\underline{m}/\underline{z}$ range of interest in the analyses;

(2) the calibration of the mass spectrometer to an "optimum" standard spectrum to adjust relative ion ($\underline{m}/\underline{z}$) abundances within specified tolerances;

(3) the minimum number of data points per chromatographic peak required to achieve acceptable precision during acquisition of full scan data;

(4) the documentation of stability of the mass spectrometer during the analysis period;

(5) the relationship between the percent standard deviation (coefficient of variation) for the relative molar response ratios as a function of the relative retention order for selected vapor-phase organics and the internal standard(s) selected for quantification;

and (6) the constancy of relative molar response ratios over the dynamic mass (quantity) range of analysis (from the limit of detection of the mass spectrometer to the overloading of the capillary column).

These factors are also discussed here.

EXPERIMENTAL METHODS

Quantitative Factors

Instrument Standardization--

The standard which has been selected for determining instrument stability as related by resolution and relative ion abundance is perfluorotoluene. Perfluorotoluene exhibits ions throughout the mass range of interest for vapor-phase organics with intensities of between 10 and 100% relative abundance. Furthermore, this compound has been routinely included as an internal standard for the quantification of vapor-phase organics in ambient air. In order to select an optimum standard spectrum, six mass spectra from samples which were analyzed on a Varian MAT CH-7 GC/MS/COMP in each of the years 1977, 1978 and 1979 were randomly chosen and an average relative intensity of each ion ($\underline{m}/\underline{z}$) in the spectrum, standard deviation, and coefficient of variation were calculated. Likewise the same concurrent information was tabulated for perfluorokerosene, a calibration standard commonly employed with magnetic sector instruments. Furthermore, six samples for the years 1978 and 1979 were selected which had been analyzed on an LKB 2091 GC/MS/COMP system. From all of these data, the average percent intensity, standard deviation and range were determined.

Precision of Loading Tenax GC Cartridges--

To measure responses as a function of concentration, the compounds of interest must be first be reproducibly loaded and desorbed from the Tenax cartridge. The loading apparatus shown in Figure 25 was used. Helium was purified by passing it through a cryogenic trap followed by two carbon traps. The sample was loaded from a methanol solution by injection through the septum of the heated loading tube. Vaporized components were swept onto the Tenax GC cartridge by the helium flow. By judiciously selecting a total purge volume of ~1.2 L, the majority of the methanol was passed through the Tenax GC cartridge and since the compounds of interest have larger breakthrough volumes they were retained on the Tenax cartridge. Thus, it was possible to load relatively non-volatile compounds, specifically those which are not amenable to preparation as permeation tubes.

To test this system, an initial set of cartridges was loaded with xylene and naphthalene using a loading tube temperature of 170°C, the Tenax cartridge temperature at 30°C, and 300 mL of helium purge volume (30 mL/min). Under these conditions, naphthalene, which was considered as representative of low vapor pressure compounds in the vapor-phase fraction, was found not to be reproducibly loaded. On the other hand, xylene was reproducibly loaded. To insure complete loading of naphthalene, the loading tube temperature was increased to 275-280°C. The Tenax GC tube temperature was 33-35°C and a helium flow of 80 mL/min for 15 min was used. Four replicate cartridges were loaded with 270 ng each of naphthalene, desorbed, and analyzed by GC on a 55 m SE-30 wide bore WCOT capillary at 120°C for 4 min and then programmed to 220°C at 4°C/min.

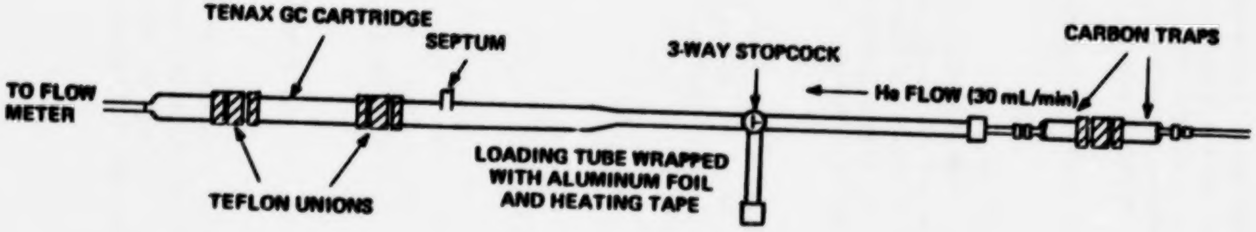

TENAX GC CARTRIDGE
SEPTUM
3-WAY STOPCOCK
CARBON TRAPS
TO FLOW METER
← He FLOW (30 mL/min)
TEFLON UNIONS
LOADING TUBE WRAPPED WITH ALUMINUM FOIL AND HEATING TAPE

Figure 25. Schematic of vaporization unit for loading organics dissolved in methanol onto Tenax GC cartridges.

RMRs vs. Relative Retention Order to Standards--

Twelve compounds - dichloromethane, 1,1-dichloroethane, perfluorobenzene, chloroform, 1,2-dichloroethane, 1,1,1-trichloroethane, carbon tetrachloride, trichloroethylene, bromodichloromethane, tetrachloroethylene, chloroform, and dichlorobenzene - were loaded as a replicate set of six on Tenax GC cartridges. Cartridges were then analyzed by thermal desorption GC/MS/COMP using an LKB 2091 system and standard conditions. A second set of six was analyzed on a Varian MAT CH-7 GC/MS/COMP system.

Data sets were statistically analyzed to obtain coefficients of variation.

RMR vs Vapor-Phase Component Quantity--

The objective of this set of experiments was to deterime whether: (1) the relative molar response ratio was constant and independent of mass quantity over the range of interest when chromatographing the vapor-phase organics on the SE-30 wide bore capillary columns; and (2) whether a mass quantity dependence might occur due to changes in sample pressure in the ion source.

Tenax GC cartridges were loaded with diethyl ether, nitromethane, 1,2-dichloroethane, n-butanol, chlorobenzene, anisole, and naphthalene at three mass quantities (~800, ~80, ~8 ng/cartridge) over the dynamic capacity range of the wide bore SE-30 coated capillaries and including near the limits of detection of the mass spectrometer. A replicate set of six cartridges for each mass level was analyzed by GC/MS/COMP and the data were statistically treated.

Qualitative and Quantitative Analysis of Ambient Air Samples

The technique for collection of vapor-phase organics has been previously described. Improvements described in this report were incorporated into the sampling and analysis protocol. These improved methods were used for the analysis of vapor-phase organics in Baton Rouge and Lake Charles, LA, Houston and Beaumont, TX.

The GC/MS/COMP analysis parameters used were identical to those described in Section 7 (Table 4).

Tables 42-45 and Figures 26-36 present the sampling protocols for Baton Rouge, Lake Charles, Beaumont and Houston and their respective sampling locations. Table 46 provides the listing of the major industrial firms in Baton Rouge, LA and vicinity depicted in Figures 26 and 27.

RESULTS AND DISCUSSION

Quantitative Factors

Instrument Standardization--

Previously recorded data accumulated on a Varian CH-7 for perfluorotoluene (PFT) and perfluorokerosene (PFK) for the years 1977, 1978 and 1979 are given in Tables 47 and 48, respectively. Included are statistics for

Table 42. SAMPLING PROTOCOL FOR BATON ROUGE, LA AND VICINITY

Site	Sampling Period/Location[a]	Sampling Time (min)	Volume Sampled (ℓ)	Remarks
Baton Rouge, LA I10 and College Dr.	P1/L5A-1,2	120	104	12/5/78 1145-1345 57°F 50% RH 180/lt.
"	P1/L5B	120	97	12/5/78 1130-1330 57°F 50% RH 180/lt.
"	P2/L5A	124	116	12/5/78 1556-1800 57°F 40% RH VAR/lt.
"	P2/L5B	119	103	12/5/78 1601-1800 57°F 40% RH VAR/lt.
"	P2/L5C	122	90	12/5/78 1558-1800 57°F 40% RH VAR/lt.
"	P3/L5A	120	114	12/5/78 1814-2014 47°F 72% RH VAR/0
"	P3/L5B	120	102	12/5/78 1815-2015 47°F 72% RH VAR/0
"	P3/L5C	120	99	12/5/78 1810-2010 47°F 72% RH VAR/0

(continued)

Table 42 (cont'd.)

Site	Sampling Period/Location[a]	Sampling Time (min)	Volume Sampled (ℓ)	Remarks	
Baton Rouge, LA Hw. 61 and Thomas Rd.	P4/L1	215	305	12/6/78 74°F 90/5 kts	1057-1432 65% RH
Baton Rouge, LA Hw. 61; Mr. E. Q. Ewell's ranch	P4/L2	120	205	12/6/78 75°F 90/lt.	1134-1334 62% RH
"	P4/L3	120	191	12/6/78 75°F 90/lt.	1150-1350 62% RH
"	P4/L4	120	192	12/6/78 75°F VAR/lt.	1210-1410 62% RH
Baton Rouge, LA Choctaw Rd. and Phlox St.	P5/L1	171	232	12/7/78 80°F 180/10 kts	0911-1202 79% RH
Baton Rouge, LA Off Route 190	P5/L2	120	190	12/7/78 80°F 180/10 kts	0940-1140 79% RH
"	P5/L3	120	189	12/7/78 80°F 180/10 kts	0952-1152 79% RH
Baton Rouge, LA Off Woodland Rd.	P5/L1	144	196	12/7/78 81°F 180/11 kts	1428-1652 77% RH

(continued)

Table 42 (cont'd.)

Site	Sampling Period/Location[a]	Sampling Time (min)	Volume Sampled (ℓ)	Remarks
Plaquemine, LA Rt. 988	P6/L2	90	123	12/7/78 1453-1623 82°F 69% RH 180/10 kts
"	P6/L3	90	141	12/7/78 1502-1632 82°F 69% RH 180/10 kts
"	P6/L4	90	157	12/7/78 1509-1639 82°F 69% RH 180/10 kts

[a] See Figures 27-29 for locations.

[b] RH = relative humidity, lt. = light, V = variable.

Table 43. SAMPLING PROTOCOL FOR VAPOR-PHASE ORGANICS IN LAKE CHARLES, LA

Site	Sampling Period/Location	Sampling Time (min)	Volume (ℓ)	Remarks	
Lake Charles, LA Off Highway 90 West & I-10	P1/L1	75	135.8	2/14/79 69°F	0835-0950 19°/10 kts
"	P2/L1	120	143.0	2/14/79 72°F	1230-1430 180°/20 kts
Lake Charles, LA Off I-210	P2/L2	120	166.1	2/14/79 72°F	1230-1430 180°/10-12 kts
Lake Charles, LA Off Highway 90 West & I-10	P3/L1	60	113.4	2/14/79 69°F	1639-1739 180°/15 kts
"	P4/L1	60	101.1	2/15/79 65°F	0904-1004 17°/12 kts
"	P5/L1	60	110.6	2/15/79 65°F	1653-1753 17°/12 kts
"	P6/L1	60	112.0	2/16/79 56°F	1419-1519 45°/5-10 kts
"	P7/L1	120	126.0	2/16/79 53°F	1443-1643 45°/5-10 kts
Lake Charles, LA Off I-210	P7/L3	120	148.4	2/16/79 52°F	1445-1645 Var/Lt.

(continued)

Table 43 (cont'd.)

Site	Sampling Period/Location	Sampling Time (min)	Volume (ℓ)	Remarks
Lake Charles, LA Off Highway 90 & I-10	P8/L1	60	101.0	2/19/79 0907-1007 34°F 270°/5-8 kts
"	P9/L1	60	103.0	2/19/79 1013-1113 36°F 270°/5 kts
"	P10/L1	60	104.0	2/19/79 1123-1223 36°F 270°/5 kts

Table 44. SAMPLING PROTOCOL FOR VAPOR-PHASE ORGANICS IN BEAUMONT, TX AND VICINITY

Site	Sampling Period/Location	Sampling Time (min)	Volume (ℓ)	Remarks	
Port Neches, TX **Spur 136 Farm Rd.**	P1/L1	2898	162.3	3/27-28/79 73°F	0955-1013 180°/10-15 kts
Beaumont, TX **West Port Arthur Rd.**	P2/L1	120	99.7	3/27/79 77°F	1240-1440 180°/10-15 kts
"	P2/L2	120	101.9	3/27/79 77°F	1240-1440 180°/10-15 kts
"	P2/L3	120	88.6	3/27/79 77°F	1240-1440 180°/10-15 kts
Groves, TX **Farm Road 366**	P3/L1	120	103.5	3/28/79 75°F	1210-1410 290°/15-20 kts
"	P3/L2	120	113.6	3/28/79 75°F	1210-1410 290°/15-20 kts
"	P3/L3	120	96.7	3/28/79 75°F	1210-1410 290°/15-20 kts
Port Neches, TX **Spur 136 Farm Rd.**	P4/L1	120	111.6	3/30/79 72°F	1135-1335 290°/10-20 kts
"	P4/L2	120	106.6	3/30/79 72°F	1135-1335 290°/10-20 kts

(continued)

Table 44 (cont'd.)

Site	Sampling Period/Location	Sampling Time (min)	Volume (ℓ)	Remarks	
Port Neches, TX Spur 136 Farm Rd.	P4/L3	120	114.7	3/30/79 72°F	1135-1335 290°/10-20 kts
Beaumont, TX Spur 380	P5/L1		102	4/3/79 63°F	1125-1325 270°/10-15 kts
"	P5/L2		98	4/3/79	1125-1325 270°/10-15 kts
"	P5/L3		121	4/3/79	1125-1325 270°/10-15 kts
FM 347	P6/L1	60	86.9	4/5/79 62°F	0945-1045 90°/5-10 kts
"	P6/L2	60	78.6	4/5/79 62°F	0945-1045 90°/5-10 kts
"	P6/L3	60	80.3	4/5/79 62°F	0945-1045 90°/5-10 kts

Table 45. AMBIENT AIR SAMPLING PROTOCOL FOR HOUSTON, TX AND VICINITY

Site	Sampling Period/Location	Sampling Time (min)	Volume (ℓ)	Remarks	
Houston, TX 16530 Pennisula Blvd.	P1/L1	90	91	6/7/79 86°F	1355-1525 210°/∿15 kts
	P2/L1	90	105	6/7/79 86°F	1545-1715 210°/∿10 kts
	P3/L1	90	89	6/8/79 86°F	940-1110 180°/5-10 kts
	P4/L1	90	76	6/8/79 82°F	1115-1245 200°/5-10 kts
	P5/L1	90	93	6/8/79 84°F	1300-1430 180°/5-10 kts
	P6/L1	90	102	6/8/79 84°F	1433-1603 210°/5-10 kts
	P7/L1	90	101	6/8/79 87°F	1606-1736 210°/10 kts
	P9/L1	90	102	6/11/79 75°F	1030-1200 45°/10-15 kts
Pasadena, TX Off Highway 225E	P9/L2	90	119	6/11/79 75°F	1000-1130 45°/10 kts
Pasadena, TX Off Richey St.	P11/L3	90	94	6/12/79 85°F	1430-1600 45°/5-10 kts
Deer Park, TX Off Highway 225E	P13/L4	90	95	6/13/79 85°F	1500-1630 45°/Lt

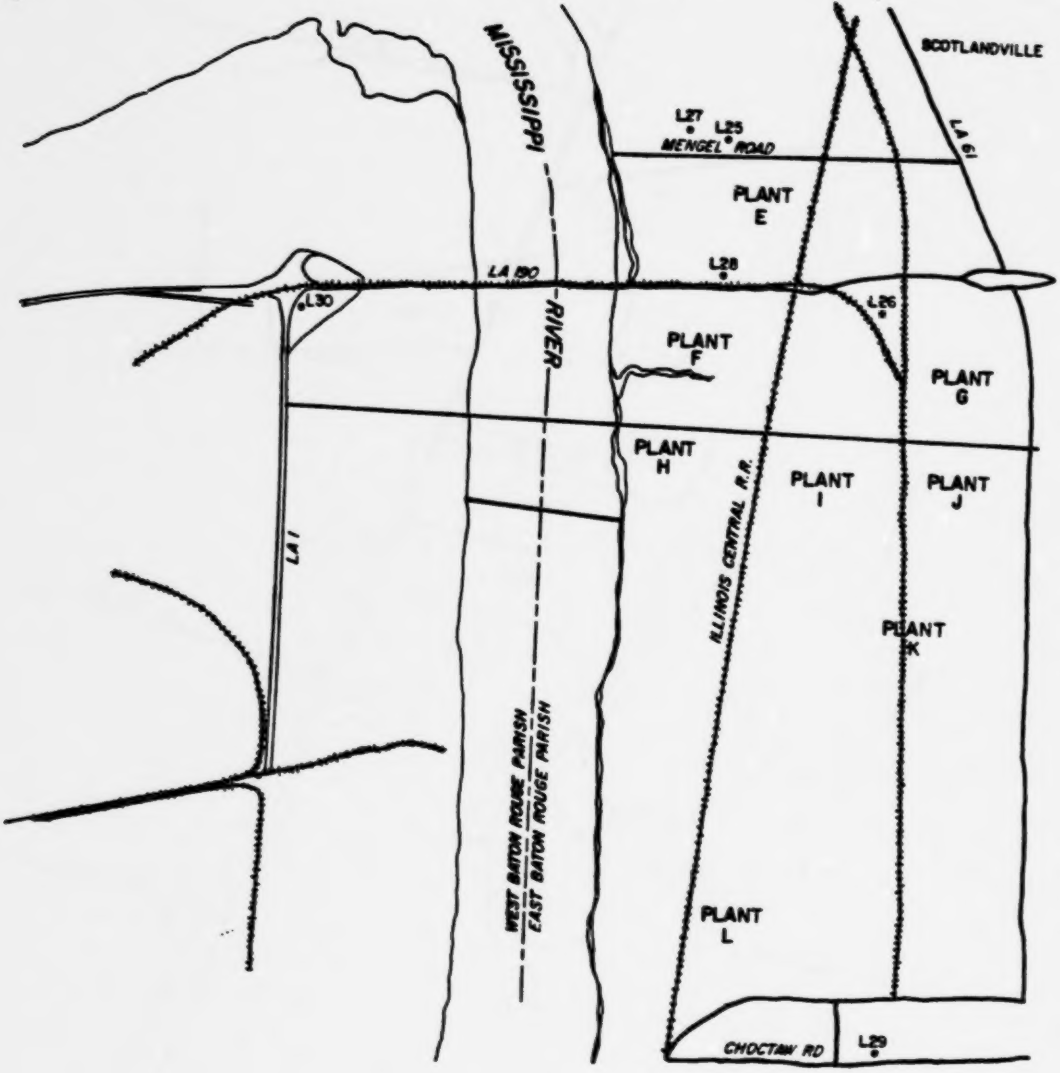

SCOTLANDVILLE
L27
L25
MENGEL ROAD
LA 61
MISSISSIPPI
RIVER
PLANT E
LA 190
L28
L30
L26
PLANT F
PLANT G
PLANT H
PLANT I
PLANT J
ILLINOIS CENTRAL R.R.
LA 1
PLANT K
WEST BATON ROUGE PARISH
EAST BATON ROUGE PARISH
PLANT L
CHOCTAW RD
L29

Figure 26. Location of plants in the East Baton Rouge Parish.

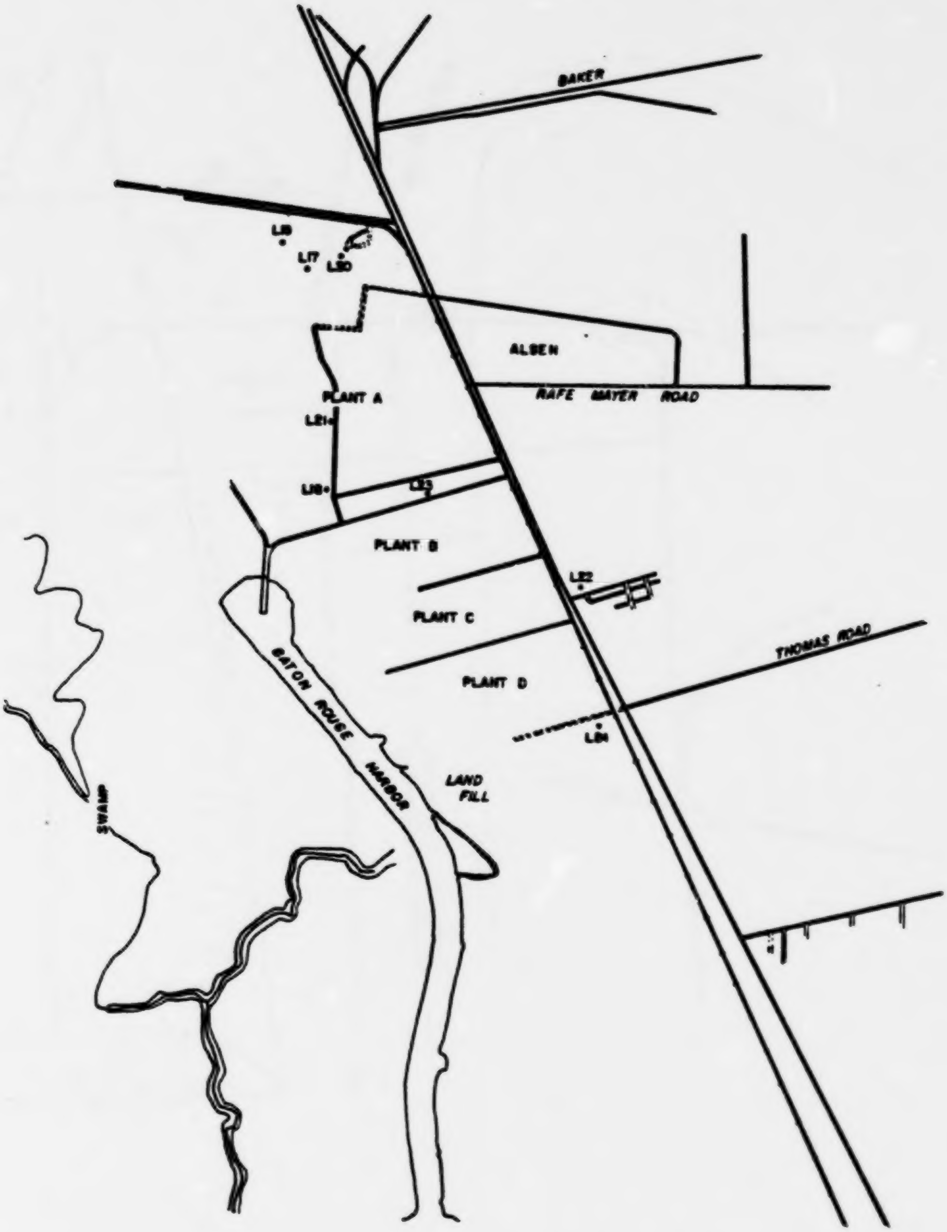

BAKER
L19
L17
L20
ALBEN
RAFE MAYER ROAD
PLANT A
L21
L18
L23
PLANT B
L22
PLANT C
THOMAS ROAD
PLANT D
L24
BATON ROUGE HARBOR
LAND FILL
SWAMP

Figure 27. Sampling locations in Baton Rouge, LA area.

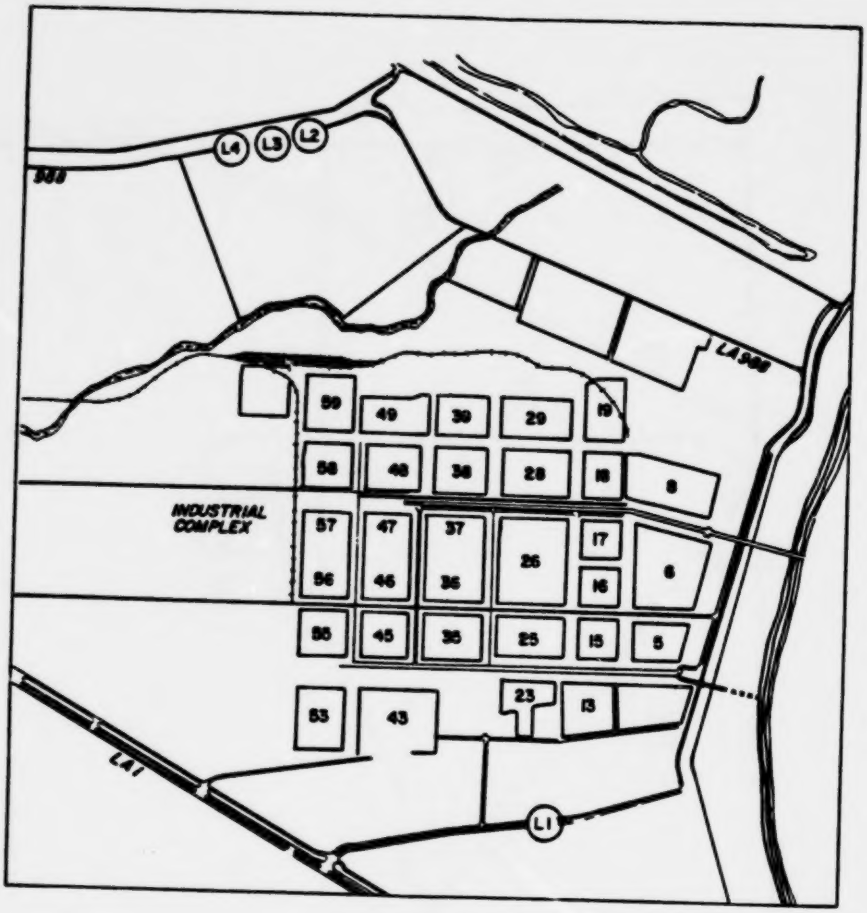

L4
L3
L2
988
LA 988
59
49
39
29
19
58
48
38
28
18
8
INDUSTRIAL COMPLEX
57
47
37
17
56
46
36
26
16
6
55
45
35
25
15
5
23
53
43
13
LA 1
L1

Figure 28. Sampling locations in Plaquemine, LA area.

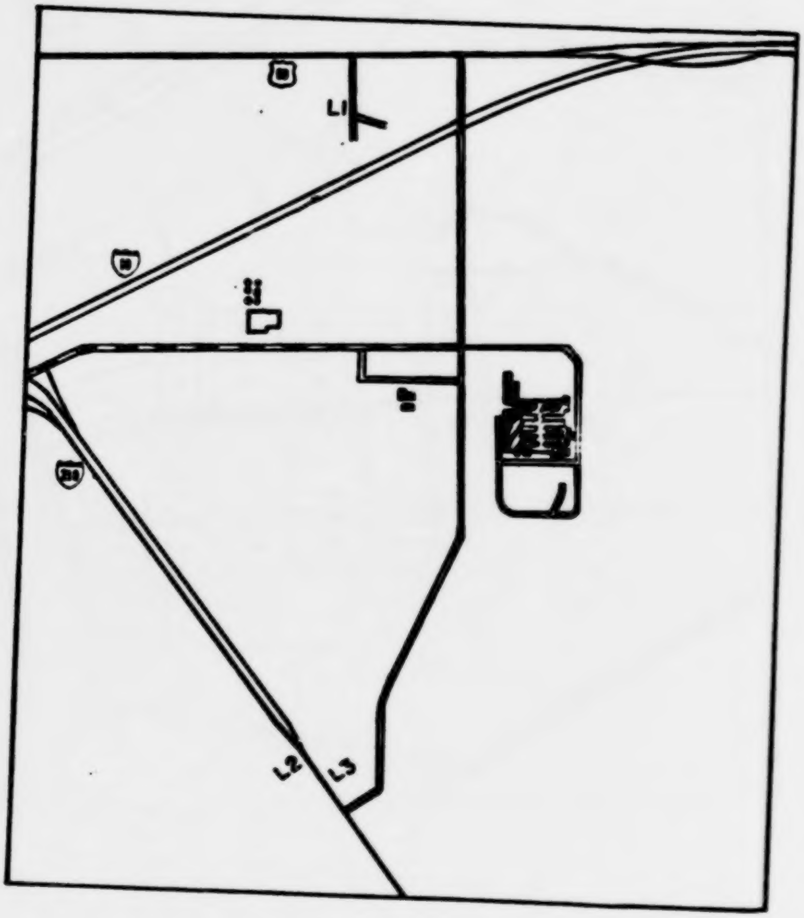


Figure 29. Sampling locations in Lake Charles, LA.

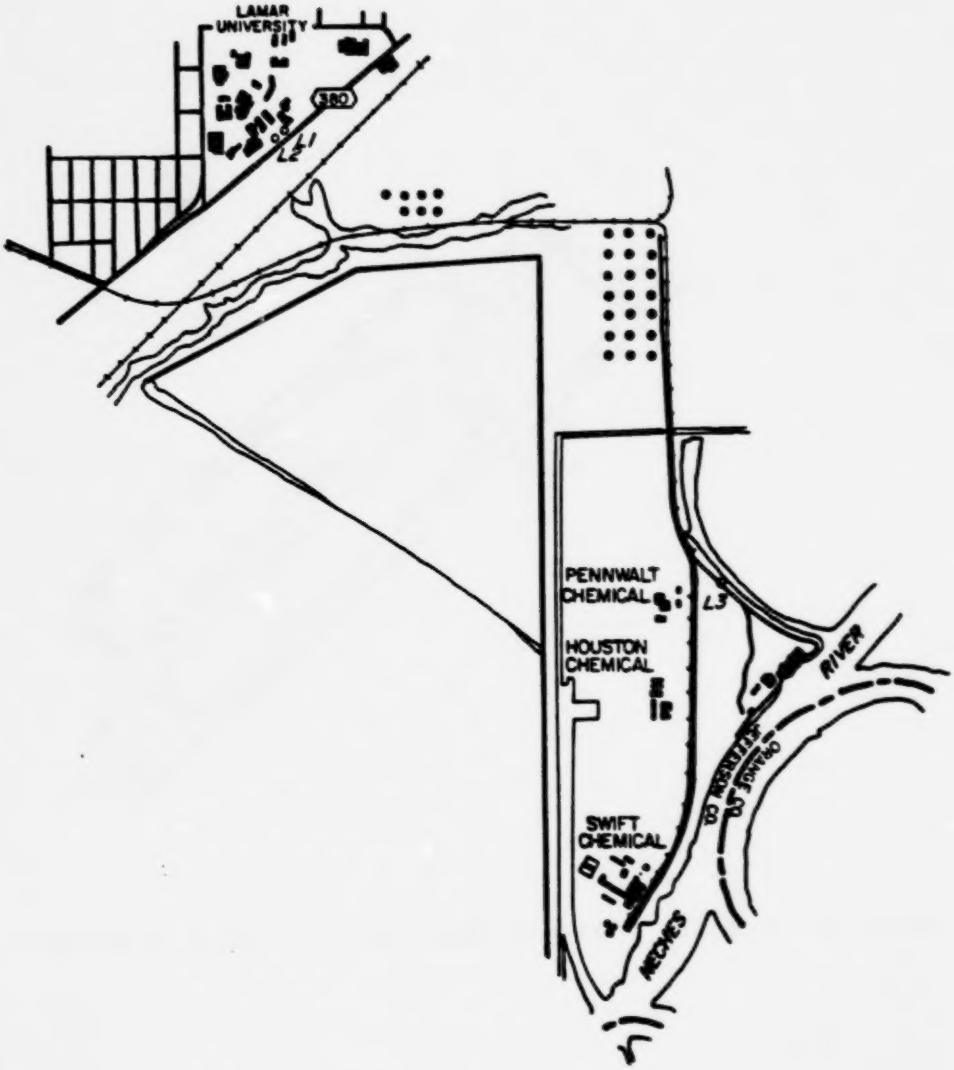

LAMAR UNIVERSITY
380
L1
L2
PENNWALT CHEMICAL
L3
HOUSTON CHEMICAL
SWIFT CHEMICAL
JEFFERSON CO
ORANGE CO
RIVER
NECHES

Figure 30. Sampling locations near Lamar University in Beaumont, TX.

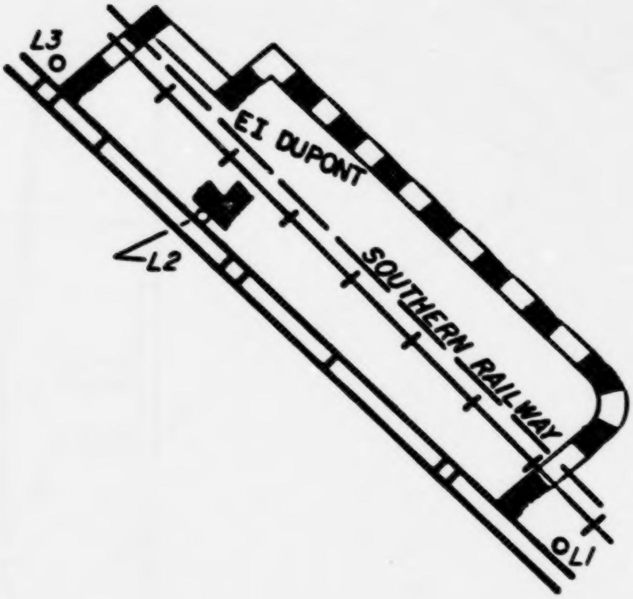

L3
EI DUPONT
L2
SOUTHERN RAILWAY
L1

Figure 31. Sampling locations along Southern Railway in Beaumont, TX.

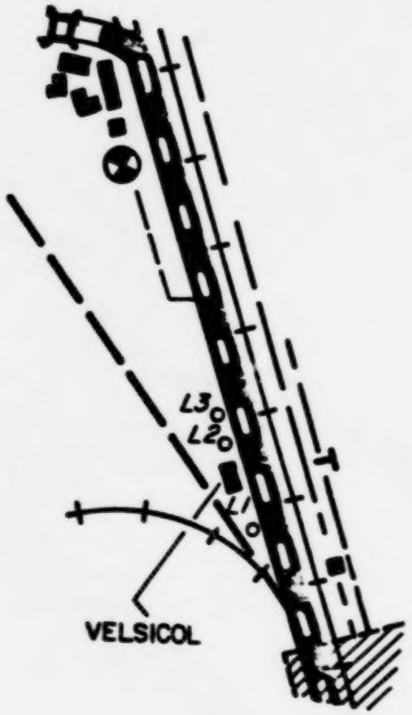

L3
L2
L1
VELSICOL

Figure 32. Sampling locations along West Port Arthur Road in Beaumont, TX.

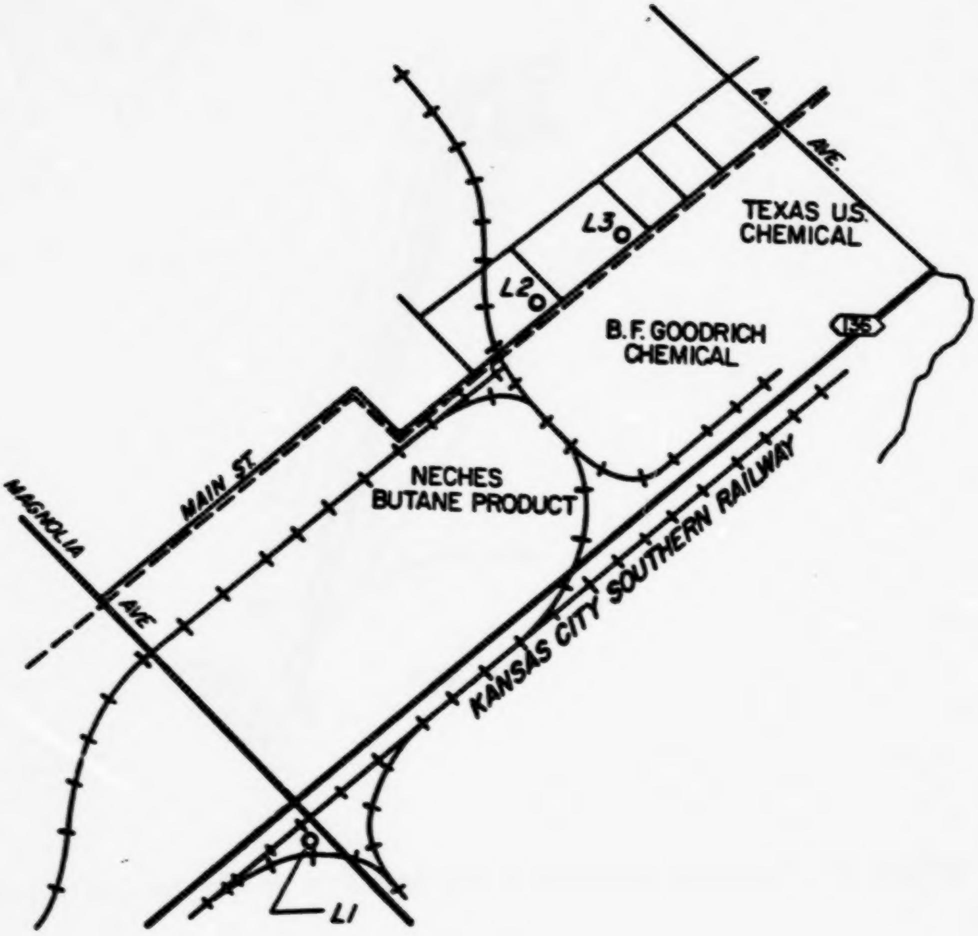
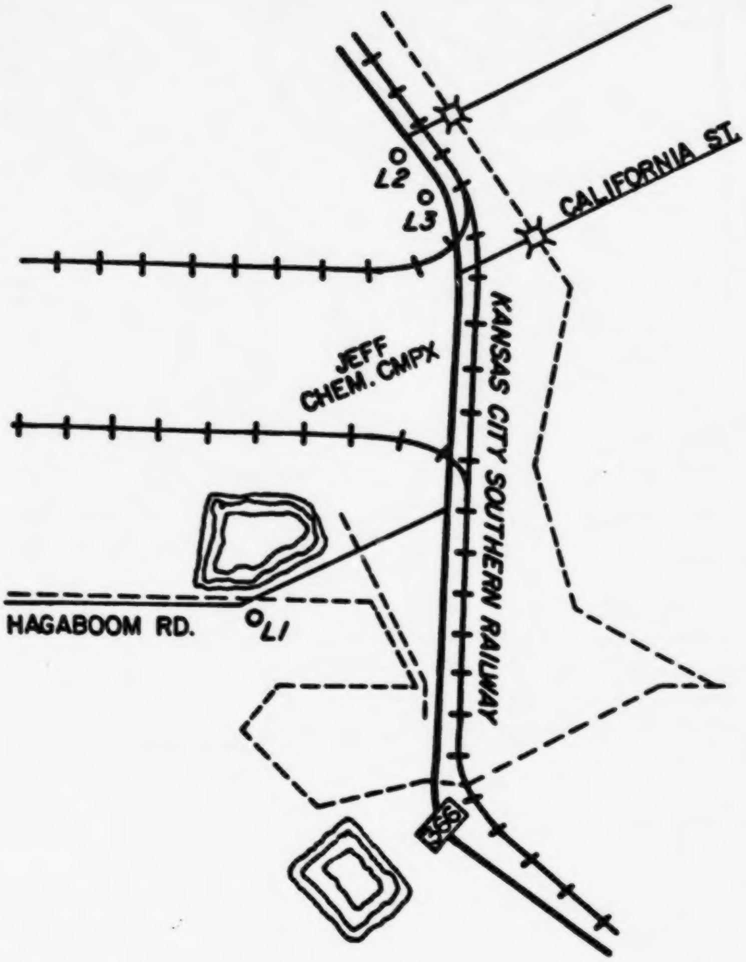

A. AVE.
TEXAS U.S. CHEMICAL
L3
L2
B.F. GOODRICH CHEMICAL
135
MAIN ST.
NECHES BUTANE PRODUCT
MAGNOLIA AVE.
KANSAS CITY SOUTHERN RAILWAY
L1

Figure 33. Sampling locations in Port Neches, TX.



CALIFORNIA ST.
L2
L3
JEFF CHEM. CMPX
KANSAS CITY SOUTHERN RAILWAY
HAGABOOM RD.
L1
366

Figure 34. Sampling locations in Groves, TX.

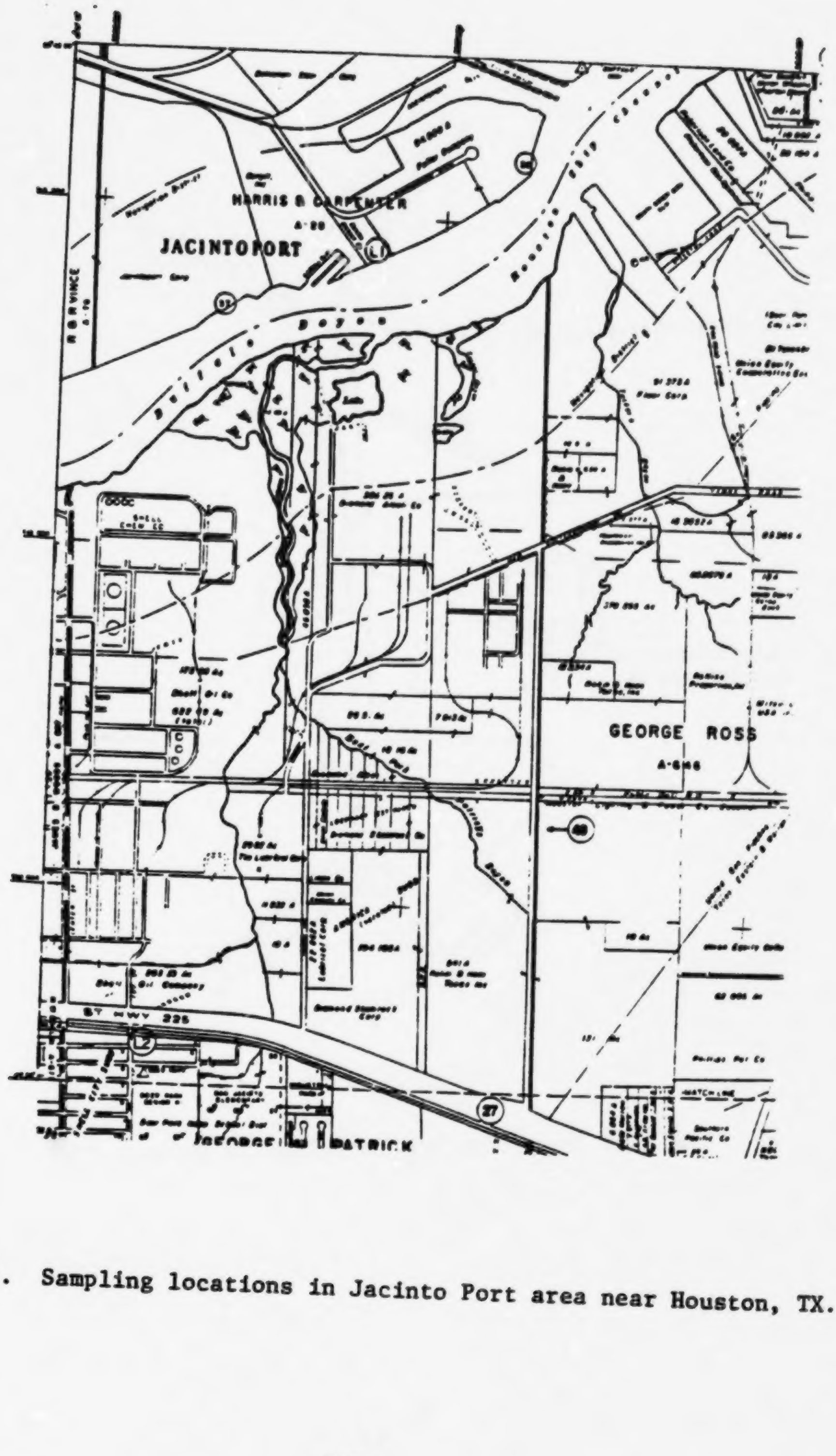

HARRIS & CARPENTER
A-80
JACINTOPORT
L1
R B R VINCE
Buffalo Bayou
GEORGE ROSS
A-646
ST HWY 225
L2
27
GEORGE
PATRICK

Figure 35. Sampling locations in Jacinto Port area near Houston, TX.

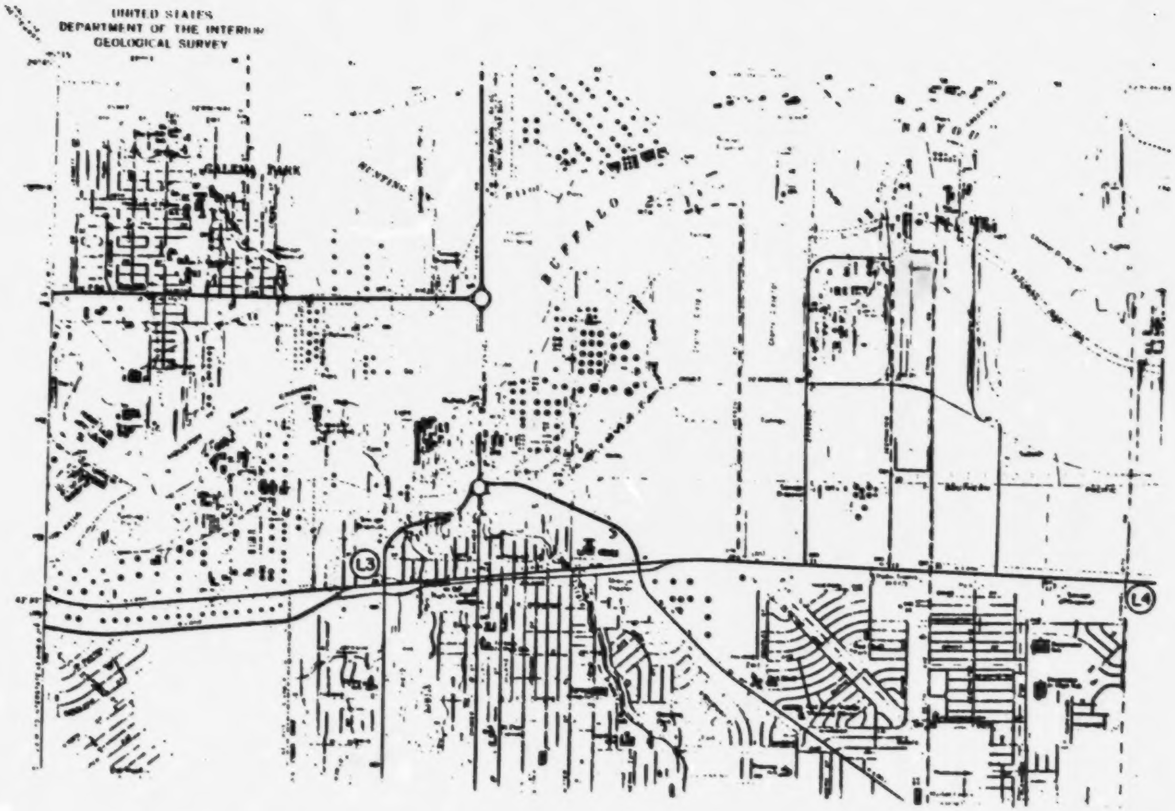

UNITED STATES
DEPARTMENT OF THE INTERIOR
GEOLOGICAL SURVEY
GALENA PARK
BUFFALO
BAYOU
L3
L4

Figure 36. Sampling locations in Deer Park and Pasadena, TX areas.

Table 46. MAJOR INDUSTRIAL PLANTS

Plant A	Rollins Environmental Services
Plant B	Allied Chemical Corporation, Plastics Plant
Plant C	Uniroyal Inc.
Plant D	American Hoechst Co.
Plant E	Stauffer Chemical Co.
Plant F	Kaiser Aluminum & Chemical Corp.
Plant G	Copolymer Rubber & Chemical Co.
Plant H	Allied Chemical North Works, Industrial Chem.
Plant I	Ethyl Corporation
Plant J	Uniroyal Inc., Gulf States Road Plant
Plant K	Exxon USA, refinery
Plant L	Allied Chemical South Works, Speciality Chem.

Table 47. RELATIVE ION ABUNDANCES FOR PERFLUOROTOLUENE OBTAINED ON A VARIAN MAT CH-7 GC/MS/COMP SYSTEM[a]

m/z	1977 %I ± S.D. (C.V.)	1978 %I ± S.D. (C.V.)	1979 %I ± S.D. (C.V.)	'77 + '78 + '79 %I ± S.D. (C.V.)
69	36 ± 17 (48)	38 ± 7.0 (18)	34 ± 2.7 (8)	36 ± 2 (5)
74	4 ± 2.1 (55)	6 ± 2.7 (45)	6 ± 1.7 (29)	5 ± 1.1 (23)
79	9 ± 4.1 (44)	14 ± 7.1 (51)	11 ± 2.2 (20)	11 ± 2.5 (23)
93	18 ± 7.3 (39)	20 ± 6.2 (31)	15 ± 1.6 (11)	18 ± 2.5 (14)
98	14 ± 5.3 (38)	11 ± 0.9 (9)	14 ± 3.1 (22)	13 ± 1.7 (13)
117	48 ± 15 (31)	47 ± 9.3 (20)	45 ± 9.7 (22)	47 ± 1.5 (3)
148	11 ± 2.4 (22)	10 ± 3.1 (31)	10 ± 1.5 (15)	10 ± 0.6 (6)
167	17 ± 1.9 (11)	18 ± 4.7 (26)	17 ± 1.9 (11)	17 ± 0.6 (4)
186	62 ± 2.8 (4)	59 ± 12 (20)	66 ± 6.3 (10)	62 ± 3.5 (6)
217	100 ± 0 (0)	100 ± 0 (0)	100 ± 0 (0)	100 ± 0 (0)
218	8 ± 0.4 (5)	8 ± 1.1 (14)	10 ± 3.0 (30)	9 ± 1.1 (13)
236	67 ± 7.2 (11)	63 ± 17 (27)	68 ± 6.1 (9)	66 ± 2.6 (4)
237	6 ± 0.8 (15)	6 ± 1.5 (25)	7 ± 1.2 (17)	6 ± 0.6 (10)

[a] Data obtained during capillary chromatography.

Table 48. RELATIVE ION ABUNDANCES FOR PERFLUOROKEROSENE OBTAINED ON A VARIAN MAT CH-7 GC/MS/COMP SYSTEM

m/z	1977	1978	1979	'77 + '78 + '79
	%I ± S.D. (C.V.)	%I ± S.D. (C.V.)	%I ± S.D. (C.V.)	%I ± S.D. (C.V.)
51	38 ± 8.0 (21)	44 ± 4.9 (11)	36 ± 4.1 (11)	39 ± 4.1 (11)
100	21 ± 3.2 (16)	21 ± 1.4 (7)	24 ± 2.1 (9)	22 ± 1.7 (8)
119[a]	100 ± 0 (0)	100 ± 0 (0)	100 ± 0 (0)	100 ± 0 (0)
131	88 ± 6.7 (8)	85 ± 2.5 (3)	95 ± 1.2 (1)	89 ± 5.1 (6)
169	60 ± 4.5 (8)	56 ± 1.7 (3)	59 ± 4.0 (7)	58 ± 2.1 (4)
181	65 ± 5.0 (8)	58 ± 6.3 (11)	62 ± 4.8 (8)	62 ± 3.5 (6)
219	26 ± 3.3 (13)	22 ± 1.0 (4)	25 ± 1.3 (5)	24 ± 2.1 (9)
231	32 ± 4.6 (15)	25 ± 1.9 (7)	29 ± 2.6 (9)	29 ± 3.5 (12)

[a] Intensities were normalized to m/z 119 since m/z 69 was saturated in all cases.

the relative ion abundances for sets of data collected during each year and then a composite data set. Variations are observed in the relative intensity of each ion (m/z) from sample to sample; however, the coefficients of variation are relatively constant when comparing data sets. No attempts had been made to "control" mass resolution and relative ion intensities for PFB when calibrating this instrument. Thus, the coefficients of variation might be expected to be larger than for a more closely "controlled" calibration. The software system on this system only tests mass resolution fits.

An "optimum" m/z vs. relative intensity listing for PFK and PFT is given in Table 49. In order to achieve a ±7% C.V. the suggested range was proposed. Use of tight relative ion intensities over the mass (m/z) range should allow the use of RMR data determined either during analysis of a sample set or from previously recorded data with a minimal variation in the RMRs.

Table 50 presents similar data obtained on an LKB-2091 for the years 1978 and 1979. In this case the software program requires mass and intensity fits to be obtained. It is very evident that the coefficients of variation are considerably better than from the CH-7 system. Concomitantly, RMR data for vapor-phase compounds have been rather constant over an extended period of time for which information exists (~ 1 year).

Precision of Loading Tenax GC Cartridges--

Results given in Table 51 indicate that naphthalene can be reproducibly loaded by the vaporization method (Fig. 25). Since the Tenax GC cartridge temperature doesn't exceed 35°C, more volatile compounds should be successfully loaded without loss. To verify this a solution of the following composition was prepared and loaded: 1,2-dichloroethane - 400 ng, nitromethane - 400 ng, toluene - 250 ng, diethyl ether - 1000 ng and naphthalene - 290 ng. Desorption and analysis by GC/MS/COMP gave the results in Table 52. Blank No. 1 was obtained by loading only a 10 µL volume of methanol. Blank No. 2 was placed in series with the cartridge tube and represents the breakthrough concentration. These data indicate that the more volatile compounds can also be loaded at the higher temperature.

An initial problem encountered with the more volatile components was that the methanol peak from the solvent was partially obscuring these components. In addition the amount of methanol that was retained on the Tenax GC cartridge was too large and interfered with the operation of the ion source in the GC/MS. It was then decided to increase the volume of helium to 1.2 L, a setting well below the breakthrough volume of the majority of compounds of interest.

RMR vs. Relative Retention Order to Standards--

Perhaps the most interesting observations were made when arranging the components in the elution order vs. the internal standard giving the lowest deviation limits under various operating conditions. Table 53 lists the coefficients of variation for RMRs as a function of relative retention order for selected vapor-phase organics. These data represent the analysis of six Tenax GC sampling cartridges which were loaded with the corresponding

Table 49. SUGGESTED MASS AND INTENSITY TOLERANCES ACCEPTABLE FOR CALIBRATION OF MAGNETIC INSTRUMENTS FOR QUANTITATION

Perfluorotoluene[a]		Perfluorokerosene	
m/z	%I (C.V.)	m/z	%I (C.V.)
69	33 (5)	51	39 (10)
79	11 (10)	100	22 (8)
93	16 (8)	119	100 (0)
117	43 (8)	131	89 (5)
167	15 (7)	169	58 (4)
186	59 (5)	181	62 (6)
217	100 (0)	219	24 (5)
236	66 (4)	231	29 (8)

[a] To be achieved in the chromatography mode.

Table 50. RELATIVE ION ABUNDANCES FOR PERFLUOROTOLUENE OBTAINED ON AN LKB-2091 GC/MS/COMP SYSTEM[a]

m/z	1978 %I ± S.D. (C.V.)	1979 %I ± S.D. (C.V.)	1978 + 1979 %I ± S.D. (C.V.)
69	30 ± 3 (10)	30 ± 1.2 (4.0)	30 ± 2.3 (7.6)
74	4 ± 0.6 (13)	5 ± 0.23 (4.0)	5 ± 0.82 (17)
79	10 ± 1.0 (10)	11 ± 1.0 (14)	11 ± 1.4 (13)
93	16 ± 1.2 (8)	17 ± 1.2 (7)	16 ± 1.3 (8)
98	12 ± 1.4 (11)	13 ± 1.8 (14)	13 ± 1.6 (12)
108	4 ± 0.38 (9)	4 ± 0.26 (6.5)	4 ± 0.37 (9)
117	37 ± 2.4 (6.8)	40 ± 2.5 (6)	39 ± 3.0 (8)
148	8 ± 0.50 (6)	9 ± 0.92 (10)	9 ± 0.73 (9)
167	13 ± 0.64 (5)	15 ± 0.78 (5)	14 ± 0.96 (7)
186	56 ± 1.4 (3)	57 ± 2.8 (5)	56 ± 2.2 (4)
217	100 ± 0 (0)	100 ± 0 (0)	100 ± 0 (0)
218	8 ± 0.42 (6)	8 ± 0.66 (8)	8 ± 0.58 (7)
236	68 ± 3.3 (5)	67 ± 1.6 (2)	67 ± 2.7 (4)
237	6 ± 0.46 (8)	6 ± 0.33 (5)	6 ± 0.39 (7)

[a] Data obtained in the chromatography mode.

Table 51. PRECISION OF LOADING NAPHTHALENE ONTO TENAX GC CARTRIDGES AND ANALYSIS BY HRGC/EIMS/COMP

Run no.	Naphthalene (ng)	Loading Temperature (°C)	Loading Volume (mL)	Peak Height
1	270	275-280	300	12.5
2	270	275-280	300	13.3
3	270	275-280	300	16.1
4	270	275-280	300	15.9
				Mean ± S.D. (C.V.) 14.4 ± 1.82 (12.6)

Table 52. PRECISION OF LOADING SELECTED VAPOR-PHASE ORGANICS ONTO TENAX GC CARTRIDGES AND ANALYSIS BY HRGC/EIMS/COMP

	Peak Height			
Run No.	Naphthalene	1,2-Dichloroethane	Nitromethane	Toluene
1	19.3	2.1	7.3	23
2	19.6	2.7	6.0	24
3	19.4	1.6	7.1	22
Mean ± S.D. (C.V.)	19.4 ± 0.15 (0.7)	2.1 ± 0.55 (26)	6.8 ± 0.7 (10)	23 ± 1 (4)
Blank 1	0.7	-	-	2.4
Blank 2	0.1	-	-	2.1

Table 53. COEFFICIENT OF VARIATION FOR RMRs AS A FUNCTION OF RELATIVE RETENTION ORDER FOR SELECTED VAPOR-PHASE ORGANICS

Compound	Relative retention	C.V.	
		Set no. 1[b]	Set no. 2[c]
Dichloromethane	0.75	5	22
1,1-Dichloroethane	0.89	5	11
Perfluorobenzene (iS)	1.00	--	--
Chloroform	1.04	8	12
1,2-Dichloroethane	1.17	3	8
1,1,1-Trichloroethane	1.19	8	12
Carbon tetrachloride	1.28	7	10
Trichloroethylene	1.44	12	12
Bromodichloromethane	1.44	13	18
Tetrachloroethylene	2.03	3	22
Chlorobenzene	2.20	13	--
Dichlorobenzene	3.06	12	--

[a] See Table 4 for instrument conditions.

[b] Data obtained using an LKB-2091 GC/MS/COMP.

[c] Data obtained using a Varian MAT CH-7 GC/MS/COMP.

compounds and then analyzed under normal operating conditions by GC/MS/COMP with an LKB-2091 system. The first set of data indicate that the coefficient of variation increased as the relative retention time to that of the internal standard perfluorobenzene also increased. For example, compare the coefficient of variation for chloroform (8%) to that of dichlorobenzene (12%). The experiment was repeated using a Varian MAT CH-7. The scan cycle times were 1.7 and 3.7 sec on the LKB 2091 and Varian CH-7 systems, respectively. The increase in the coefficient of variation between the two systems is evident since the number of data points generated per chromatographic peak on the LKB 2091 was greater than the Varian CH-7 since the average resident time of a chromatographic peak is ~6-8 sec on wide bore capillaries. It appeared that a minimum of 5 data points (scans) was necessary to adequately describe the chromatographic peak using the reconstructed total ion current obtained from full scan data. These data suggest that a second standard is required which elutes in the chromatographic range near chlorobenzene/naphthalene to obtain the highest precision.

The observations described here have been thoroughly studied and also reported elsewhere (10).

RMR vs. Vapor-Phase Component Quantity--

Experiments were conducted in order to determine whether or not relative molar response values of vapor-phase organics analyzed by GC/MS/COMP were independent of mass over the dynamic range of interest. Since the RMR value is ultimately based upon a response/molecule, it should be mass quantity independent. An observed dependence of RMR values on mass may occur, *e.g.*, due to adsorptive losses on the chromatographic column which would then inherently negate the validity of the assumption. The use of relative molar response ratios is based upon a one point calibration curve with a *required* linearity over the entire range of interest and an intercept through zero. A dependence on mass due to, for example, changes in sample pressure in the ion source would, however, also negate the assumption of a constant RMR. This question therefore is a major one which must be answered positively if the concept of RMR is to be used as a means of obtaining quantitative information with a GC/MS/COMP system.

The compounds selected for the study of the effect of concentrations on the relative molar response ratio are shown in Table 54. Diethyl ether, anisole, chlorobenzene, 1,2-dichloroethane, nitromethane, naphthalene, *p*-xylene and toluene were chosen because they represent vapor-phase organics which are typical of the classes that have been detected in the ambient air. These compounds were loaded at three concentration levels over two orders of magnitude and six replicates were run at each loading level. The analyses were run on an LKB 2091 using a 75 m SE-30 wide bore WCOT capillary (Table 4). Relative molar response ratios relative to perfluorobenzene were determined by peak heights. These results are shown in Table 54. These data show remarkable consistency over a concentration of two orders of magnitude. The coefficients of variation are comparable with those found in other experiments and the errors involved include those encountered in loading, desorption and analysis. It should be pointed out that the lowest concentration of the three is quite close to the detection limit of the mass spectrometer for all compounds under these operating conditions.

Table 54. PRECISION OF RELATIVE MOLAR RESPONSE RATIO
AS A FUNCTION OF MASS OF COMPOUND

Compound	*m/z*	Quantity (ng)	RMR ± S.D. (C.V.)
Diethyl ether	59	842	0.36 ± 0.036 (10)
		84.2	0.36 ± 0.188 (52)[b]
		8.4	0.35[a] ---
			Mean 0.36 ± 0.012 (3)
Nitromethane	61	800	0.14 ± 0.044 (31)
		80	0.13 ± 0.016 (12)
		8	0.17[a] --
			0.15 ± 0.021 (14)
1,2-Dichloroethane	62	800	0.65 ± 0.046 (7)
		80	0.71 ± 0.036 (5)
		8	0.79 ± 0.130 (16)
			0.73 ± 0.21 (28)
n-Butanol	56	800	0.33 ± 0.073 (22)
		80	0.32 ± 0.068 (21)
		8	--[a]
			0.32 ± 0.070 (21)
Chlorobenzene	112	800	1.39 ± 0.07 (5)
		80	1.19 ± 0.13 (11)
		8	2.03 ± 0.35 (17)
			1.65 ± 0.47 (28)
Anisole	108	800	0.96 ± 0.055 (6)
		80	0.85 ± 0.049 (6)
		8	0.92 ± 0.115 (12)
			0.91 ± 0.094 (10)
Naphthalene	128	750	1.51 ± 0.19 (12)
		75	1.51 ± 0.47 (31)
		7.5	1.94 ± 0.59 (30)
			1.65 ± 0.51 (30)

[a] Near or below limit of detection.

[b] May result from a poor loading of one sampling cartridge.

Use of Deuterated Compounds During Ambient Air Sampling

It is recommended that, during ambient air sampling, deuterated compounds be incorporated into the sampling regime. There is a high probability that deuterated organics will not be found in ambient air and thus they will not interfere with the subsequent analysis. The mass spectrometer provides an ability to differentiate between deuterated compounds which are considered exogenous as compared to the endogenous vapor-phase organics in ambient air.

The incorporation of deuterated compounds can be performed in two ways: (1) a series of deuterated compounds [e.g., d_6-dimethylamine, d_6-benzene, d_5-bromoethane, d_{10}-cyclohexene and d_8-styrene may be loaded as a discrete zone directly onto the Tenax GC sampling cartridge using the vaporization system depicted in Figure 21 or from permeation tubes; and (2) by the use of permeation tubes during field sampling whereby the ambient air stream is spiked with known quantities.

The use of deuterated compounds in the sampling regime provides an ability to check on potential artifacts which may occur as a result of the reactivity of the atmosphere being sampled. The suggested deuterated compound would allow for determination whether nitrosation, ozonization or halogenation might have occurred during the concentration of organics onto the sampling cartridges, since the mass spectrometer provides the opportunity to identify any deuterated by-products. Furthermore the incorporation of the suggested deuterated compounds provides a check on the breakthrough volumes which have been calculated for a series of compounds of interest in order to quantify them. Any variations in the breakthrough volume of a compound as a direct result of the specific air sampled would be reflected by these compounds since they span a large range of breakthrough volumes that are experienced for vapor-phase compounds. The premature disappearance of these compounds would indicate that the quantity of air sampled is beyond the dynamic range of the collection device (i.e., capacity which exists as a function independent of frontal displacement chromatography). A standard technique used by most laboratories employs backup sampling cartridges to determine whether premature breakthrough of organic constituents has occurred. Although this technique has been employed in the quantification of vapor-phase organics by GC/MS/COMP, the use of deuterated compounds as suggested above is preferred. The use of a backup cartridge alters the pressure differential across a sampling device and thus complicates the determination of premature breakthrough since vacuum stripping of adsorbed materials also becomes a factor leading to premature breakthrough.

Statistical Analysis of Permeation Rates

In previous reports, research has been described in the development of a permeation system and the use of permeation tubes for the purpose of calibrating the GC/MS/COMP system for quantification of vapor-phase organics in ambient air samples. Procedures have employed the weekly to biweekly gravimetric determinations of the weight losses of permeation tubes to calculate the permeation rate for each organic compound. A statistical approach has been developed in this laboratory which utilizes a linear regression analysis of the six most recent gravimetric determinations for each permeation tube. The permeation rate calculated on this basis thus has associated with it an error band (standard deviation). Permeation rates which exhibit percent standard deviations of >10% or a significant non-zero slope are rejected for purposes of calibrating the GC/MS/COMP systems.

Qualitative and Quantitative Analyses

The vapor-phase organics which were identified in ambient air from Baton Rouge, Plaquemine and Lake Charles, LA, Beaumont, Groves, Port Neches, Houston, Deer Park and Pasadena, TX are given in Appendix A.

Many of the halogenated hydrocarbons which have been previously identified during sampling trips executed between the period of 1973 to 1977 were again identified in these samples. The site-specific and ubiquitous halogenated hydrocarbons were again detected in these atmospheres. Tables 55-57 present the estimated levels of several of these vapor-phase organics.

Several levels of compound identification have been employed in the course of analysis of vapor-phase organics in ambient air samples. These criteria have developed throughout several years of experience in the identification of organic compounds and have been used in our laboratories to establish the degree of certainty of the identity of an organic compound. These levels of identification are as follows:

Level I Computer Interpretation. The raw data generated from the analysis of samples are subjected to computerized deconvolution/library search and compound identification made using this approach has the lowest level of confidence. In general Level I is reserved for only those cases where compound verification is the primary intent of the qualitative analysis.

Level II Manual Interpretation. The plotted mass spectra are manually interpreted by a skilled interpretor and compared to those spectra compiled in a data compendium. In general a minimum of five masses and intensities (±5% S.D.) should match between the unknown and library spectrum. This level does not utilize any further information such as retention time since many compounds the authentic compound may not be available for establishing retention times.

Level III Manual Interpretation Plus Retention Time/Boiling Point of Compound. In addition to the effort as described under Level II, the retention time of the compound is compared to the retention time which has been derived from previous chromatographic analysis. Also the boiling point of the identified component is compared to the boiling points of other compounds in the near vicinity of the one in question when a capillary coated with a non-polar phase has been used.

Table 55. ESTIMATED LEVELS OF SEVERAL VAPOR PHASE ORGANICS IN LAKE CHARLES, LA AIR[a]

Chemical	Sample Code			
	P2/L1-T1	P2/L2-T1[b]	P7/L1-T_1[b]	P7/L3-T_1
Benzene	223	223	217	867
Vinylidene chloride	51	ND	ND	6,226
Chloroform	118	107	96	862
Carbon tetrachloride	46	44	46	107
1,2-Dichloroethane	66	47	1,309	11,516
1,1,1-Trichloroethane	98	69	67	1,739
Trichloroethylene	45	29	61	9,557
Tetrachloroethylene	50	40	69	3,504
Dichlorobenzene isomer	6	6	5	13
Dichlorobenzene isomer	T	2	T	12
1,2-Dichloroethylene	ND	ND	ND	8,233
1,2-Dichloroethylene	ND	ND	ND	8,240
1,1,2-Trichloroethane	ND	ND	53	3,632
1,1,1,2-Tetrachloroethane	ND	ND	ND	741
Chlorobenzene	ND	T	8	40
1,1,2,2-Tetrachloroethane	ND	ND	64	4,946
1,3,5-Trichlorobenzene	ND	ND	ND	8
Pentachloroethane	ND	ND	ND	273
Pentachlorobromoethane	ND	ND	ND	347
Pentachlorobutadiene	ND	ND	ND	713
Hexachlorobutadiene	ND	ND	ND	1,312
Bromoform	ND	ND	ND	ND
Bromocyclohexane isomer	ND	ND	ND	ND
Chloromethylbutene isomer	ND	ND	ND	ND

[a] See Table 43 for sampling protocol.

[b] Upwind sample, all values in ng/m^3.

Table 56. ESTIMATED LEVELS OF ORGANIC VAPOR-PHASE POLLUTANTS IN AMBIENT AIR OF BEAUMONT, TX AND VICINITY[a]

Compound	Period/Location														
	P2/L1	P2/L2	P2/L3	P3/L1	P3/L2	P3/L3	P4/L1	P4/L2	P4/L3	P5/L1	P5/L2	P5/L3	P6/L1	P6/L2	P6/L3
Ethyl acetate	133	258 ± 91	100	8,200	T	681 ± 252	3,649	583	4,140	9,323	4,140	T	ND	1,840 ± 5	T
Benzene	4,239	5,119 ± 1,554	2,935	14,630	913	1,478 ± 304	7,783	3,065	33,848	8,348	6,326	3,000	4,413	2,478 ± 217	6,130
1,2-Dichloropropane	T	ND	ND	ND	2,347	1,459 ± 0	ND	T	ND	T	ND	T	ND	ND	T
Tetrachloroethylene	250	532 ± 139	202	820	204	790	884	449	925	2,960	620	496	334	303 ± 8	750
Chlorobenzene	90	319 ± 55	90	70	124	1,190	62	93	84	80	T	T	ND	ND	T
Carbon tetrachloride	555	666 ± 55	833	1,500	611	749 ± 194	944	772	833	16,389	722	1,000	772	1,639 ± 250	3,111
1,2-Dibromoethane	T	T	ND	ND	ND	T	T	ND	T	1,600	1,390	T	ND	ND	T

[a] See Table 44 for sampling protocol.

Table 57. ESTIMATION OF LEVELS OF VAPOR-PHASE ORGANICS IN AMBIENT AIR IN HOUSTON, DEER PARK AND PASADENA, TX AND VICINITY[a]

Compound	Period/Location									
	P1/L1	P3/L1A	P3/L1B	P4/L1	P5/L1	P6/L1	P9/L1	P9/L2	P11/L3	P13/L4
1,2-Dichloroethane	26,100 ± 4,000	7,225 ± 1,025	5,825 ± 1,925	4,200 ± 600	13,450	11,050 ± 600	900	7,750	T	700
1,1,1-Trichloroethane	620 ± 100	900 ± 140	980 ± 140	1,140 ± 100	760	1,360 ± 520	1,360	560	720	600
Carbon tetrachloride	5,266 ± 1,533	1,767 ± 100	1,566 ± 33	867 ± 0	933	933 ± 133	800	6,600	1,467	T
Trichloroethylene	2,433 ± 600	1,367 ± 0	1,383 ± 183	650 ± 150	567	567	T	3,333	3,833	ND
Bromodichloromethane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Dibromochloromethane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Tetrachloroethylene	15,862 ± 3,567	23,404	12,107 ± 3,219	2,112 ± 125	1,330	1,420 ± 50	140	2,269	957	606
Chlorobenzene	T	640 ± 123	477 ± 241	2,796 ± 335	1,300	900 ± 40	T	84	T	149
Dichlorobenzene isomer	67	T	T	T	T	T	ND	ND	T	191
Dichlorobenzene isomer	76	T	T	T	ND	80	ND	T	ND	ND
Hexachlorobutadiene	318 ± 32	416	404 ± 134	237	T	220	ND	T	ND	ND

[a] See Table 45 for sampling protocol.

Level IV Manual Interpretation Plus Retention Time of Authentic Compounds. Under this Level, the authentic compound has been chromatographed on the same capillary column using identical operating conditions and the mass spectrum of the authentic compound is compared to that of the unknown.

Level V Level IV Plus Independent Confirmation Techniques. This Level utilizes other physical methods of analysis such as GC/fourier transform/IR, GC/high resolution mass spectrometry, or NMR analysis. This Level constitutes the highest degree of confidence in the identification of organic compounds.

The predominant qualitative analysis that has been performed during the past several years has utilized Level III for qualitative analysis.

Appendix B gives the profile listings for the halogenated compounds identified. Many of these have been suggested as potential atmospheric carcinogens.

SECTION 9

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APPENDIX A

VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR

Part I	Baton Rouge and Plaquemine, LA and Vicinity
Part II	Lake Charles, LA and Vicinity
Part III	Beaumont, Orange, Groves, and Neches, TX
Part IV	Houston, Deer Park, and Pasadena, TX

Part I - BATON ROUGE AND PLAQUEMINE, LA

Table A1. "PURGEABLE" ORGANICS IDENTIFIED IN A WATER SAMPLE FROM BATON ROUGE, LA AREA (P4/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	41	$N_2 + O_2$
2	42	CO_2
3	44	$CF_2Cl_2 + C_4H_8$ isomer
4	46	acetaldehyde
5	52	$CFCl_3$
6	54	*n*-pentane
7	55	acetone
8	56	dichloromethane
9	57	Freon 113
10	60	*t*-butanol
10A	62	C_6H_{14} isomer (tent.)
10B	64	C_6H_{14} isomer
11	67	hexafluorobenzene (eS)
12	68	*n*-hexane
13	69	chloroform
14	72	perfluorotoluene (eS)
14A	73	C_6H_{12} isomer
15	78	benzene
15A	79	cyclohexane
16	82	C_7H_{16} isomer
17	88	C_7H_{16} isomer
18	92	methylcyclohexane
19	95	dimethyl disulfide
20	98	$C_6H_{12}O$ isomer
21	100	toluene
22	102	C_8H_{18} isomer
23	108	*n*-octane
24	113	hexamethylcyclotrisiloxane
25	117	chlorobenzene
26	122	ethylbenzene
27	125	C_9H_{20} isomer
28	126	$C_{10}H_{22}$ isomer
29	129	C_9H_{20} isomer
30	132	$C_{10}H_{22}$ isomer
31	136	sat. hydrocarbon
32	137	unsat. hydrocarbon
33	142	$C_{10}H_{22}$ isomer
33A	143	benzaldehyde
34	144	$C_{10}H_{22}$ isomer
35	148	*n*-decane
36	149	dichlorobenzene isomer
36A	151	$C_{11}H_{24}$ isomer
37	153	$C_{11}H_{24}$ isomer
38	155	$C_{11}H_{24}$ isomer
38A	155	$C_{11}H_{22}$ isomer
39	156	$C_{11}H_{24}$ isomer
40	159	sat. hydrocarbon
40A	161	acetophenone
40B	163	*n*-nonanal (tent.)
40C	165	$C_{11}H_{24}$ isomer
40D	170	$C_{12}H_{26}$ isomer
41	174	unknown
42	179	trichlorobenzene isomer
43	186	unsat. hydrocarbon (tent.)
44	219	unknown

[a] See Table 42 for protocol.

Table A2. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM BATON ROUGE, LA AREA (P4/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
3	48	isobutane
3A	49	C_4H_8 + chloroethylene (tent.) isomers
3B	49	n-butane
4	50	acetaldehyde
5	52	C_4H_8 isomer
6	55	isopentane
7A	57	furan + C_5H_{10} isomer
8	58	acetone + n-pentane
9	59	C_5H_{10} isomer
9A	60	methylene chloride
10A	64	ethylamine (tent.)
11	66	t-butanol
11A	67	C_5H_{10} isomer
12	67	2-methylpentane
13	70	3-methylpentane
14	71	C_6H_{12} isomer
14A	71	n-butanal
14B	72	hexafluorobenzene (eN)
15	73	n-hexane
15A	74	C_6H_{12} isomer
15B	74	chloroform
16	74	methyl ethyl ketone
17	76	ethyl acetate
17A	77	C_7H_{16} isomer
18	78	perfluorotoluene (eN) + methylcyclopentane
18A	80	1,2-dichloroethane
19	80	1,1,1-trichloroethane
19A	83	C_7H_{14} isomer
20	84	benzene
20A	85	carbon tetrachloride
21	85	cyclohexane
22	86	C_7H_{16} isomer
22A	87	2,3-dimethylpentane
23	88	3-methylhexane
23A	90	C_7H_{14} isomer
24	91	C_7H_{14} isomer
24A	91	C_8H_{18} isomer + trichloroethylene
25	93	n-heptane
25A	95	acetic acid
25B	96	2-methyltetrahydrofuran
26	99	methylcyclohexane
26A	100	C_8H_{18} isomer
26B	101	C_8H_{18} isomer
26C	102	4-methyl-2-pentanone
27	103	cyanobutadiene
28	104	4-pentene nitrile
28A	107	toluene
29	108	1-cyano-1-butene
29A	110	C_8H_{18} isomer
29B	111	C_8H_{16} isomer
30	113	C_8H_{16} isomer
31	116	n-octane
32	117	tetrachloroethylene
32A	120	C_9H_{20} isomer
32B	122	C_9H_{20} isomer
33	123	4-vinylcyclohexane
33A	124	C_8H_{16} isomer
34	125	C_6H_9N isomer (tent.)
35	128	ethylbenzene
36	130	m- and/or p-xylene
37	132	C_9H_{20} isomer
38	133	$C_8H_{18}O$ isomer (tent.)
38A	134	C_9H_{20} isomer
39	134	styrene
40	135	o-xylene
40A	136	C_9H_{18} isomer
41	137	n-nonane
42	141	isopropylbenzene + $C_{10}H_{22}$ isomer
43	143	$C_{10}H_{22}$ isomer
43A	144	$C_{10}H_{20}$ isomer
44	145	propylcyclohexane + $C_{10}H_{22}$ isomer
44A	146	$C_{10}H_{20}$ isomer
44B	146	$C_{10}H_{16}$ isomer
44C	147	$C_{10}H_{20}$ isomer
44D	147	chlorotoluene isomer
45	148	n-propylbenzene
46	148	benzaldehyde
47	149	m- and/or p-ethyltoluene
47A	150	$C_{10}H_{22}$ isomer
47B	150	1,3,5-trimethylbenzene
48	151	$C_{11}H_{24}$ isomer
48A	151	$C_{10}H_{20}$ isomer
49	152	$C_{10}H_{22}$ isomer
50	153	o-ethyltoluene
51	153	$C_{11}H_{24}$ isomer
51A	154	$C_{11}H_{24}$ isomer

(continued)

Table A2 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
52	155	$C_{10}H_{20}$ isomer
53	156	1,2,4-trimethylbenzene
53A	156	$C_{10}H_{20}$ isomer
54	157	*n*-decane
55	159	benzyl chloride + C_4-alkyl benzene isomer
55A	159	C_4-alkyl benzene isomer
55B	159	$C_{11}H_{24}$ isomer
55C	160	$C_{12}H_{24}$ isomer
56	161	$C_{11}H_{24}$ isomer
57	162	$C_{11}H_{24}$ isomer + 1,2,3-trimethylbenzene
58	163	$C_{12}H_{26}$ isomer
58A	164	dichlorobenzene isomer (trace)
58B	164	indan
59	165	butylcyclohexane + $C_{11}H_{24}$ isomer
59A	165	$C_{11}H_{22}$ isomer
59B	166	C_4-alkyl benzene isomer
60	166	$C_{11}H_{24}$ isomer
61	167	C_4-alkyl benzene isomer
61A	167	$C_{11}H_{22}$ isomer
61B	168	$C_{11}H_{24}$ isomer
62	169	acetophenone
63	169	$C_{11}H_{24}$ isomer
64	170	$C_{12}H_{26}$ isomer
64A	171	C_4-alkyl benzene isomer
65	173	$C_{11}H_{24}$ isomer
65A	173	unsat. hydrocarbon
66	174	$C_{11}H_{22}$ isomer
66A	175	$C_{11}H_{20}$ isomer
67	176	*n*-undecane
68	177	$C_{11}H_{22}$ isomer
68A	178	$C_{11}H_{20}$ isomer
69	179	$C_{12}H_{26}$ isomer
69A	180	C_4-alkyl benzene isomer
69B	180	unsat. hydrocarbon
70	181	$C_{12}H_{26}$ isomer
70A	181	$C_{11}H_{20}$ isomer
70B	182	$C_{12}H_{24}$ isomer
70C	183	unsat. hydrocarbon
71	184	C_5-alkyl cyclohexane isomer
71A	184	$C_{11}H_{22}$ isomer
71B	185	$C_{12}H_{24}$ isomer
72	186	$C_{12}H_{26}$ isomer
73	186	$C_{12}H_{26}$ isomer
74	187	$C_{12}H_{26}$ isomer
74A	188	$C_{12}H_{24}$ isomer
75	188	$C_{12}H_{26}$ isomer
75A	189	C_5-alkyl benzene isomer (traces)
75B	190	trichlorobenzene isomer (traces)
75C	190	$C_{12}H_{22}$ isomer
76	191	naphthalene
77	192	*n*-dodecane
77A	194	$C_{12}H_{22}$ isomer
77B	194	$C_{12}H_{24}$ isomer
78	195	$C_{13}H_{28}$ isomer
79	196	unsat. hydrocarbon
79A	198	$C_{13}H_{26}$ isomer
79B	198	$C_{13}H_{28}$ isomer
79C	199	$C_{13}H_{26}$ isomer
79D	200	C_6-alkyl cyclohexane isomer
79E	200	$C_{13}H_{28}$ isomer
79F	202	$C_{14}H_{30}$ isomer
79G	202	$C_{13}H_{28}$ isomer
79H	203	$C_{13}H_{26}$ isomer
79I	204	$C_{14}H_{30}$ isomer
79K	208	$C_{13}H_{26}$ isomer
80	209	*n*-tridecane
80A	210	β-methylnaphthalene
80B	211	$C_{14}H_{30}$ isomer
80C	212	α-methylnaphthalene
80D	213	$C_{15}H_{32}$ isomer
80E	215	$C_{14}H_{28}$ isomer
80F	216	$C_{14}H_{30}$ isomer
80G	217	$C_{15}H_{32}$ isomer
80H	218	unsat. hydrocarbon
80I	220	$C_{15}H_{32}$ isomer (traces)
80J	221	biphenyl (traces)
80K	221	$C_{14}H_{28}$ isomer
81	223	*n*-tetradecane
81A	225	unsat. hydrocarbon
81B	239	$C_{15}H_{32}$ isomer

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[a] See Table 42 for protocol.

Table A3. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM BATON ROUGE, LA AREA (P4/L4)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
	41	$H_2 + O_2$
1	42	CO_2
2	44	isobutane
2A	46	C_4H_8 isomer
2B	46	*n*-butane
3	47	acetaldehyde
3A	47	C_4H_8 isomer
4A	50	isopentane
5A	52	*n*-pentane
6	53	acetone
7	55	dichloromethane
9	61	2-methylpentane
9A	62	C_5H_{10} isomer
10	63	3-methylpentane
11	64	C_6H_{12} isomer + butanal (tent.)
12	64	hexafluorobenzene (eS)
13	65	*n*-hexane
14	68	ethyl acetate
15	70	perfluorotoluene (eS)
16	70	methylcyclopentane
16A	71	C_7H_{16} isomer
17	72	1,1,1-trichloroethane
17A	74	C_7H_{14} isomer
18	75	benzene
18A	76	carbon tetrachloride (traces)
19	77	cyclohexane
20	78	2-methylhexane
21	80	3-methylhexane
21A	82	C_7H_{14} isomer
22	83	C_7H_{14} isomer
23	85	*n*-heptane
24	90	methylcyclohexane
24A	91	C_8H_{16} isomer
25	92	C_8H_{16} isomer
26	98	toluene
27	99	C_8H_{18} isomer
28	101	C_8H_{18} isomer
28A	103	C_8H_{16} isomer
29	107	*n*-octane
30	109	tetrachloroethylene
32	114	4-vinylcyclohexene
33	119	ethylbenzene
34	121	*m*- and/or *p*-xylene
35	123	C_9H_{20} isomer
35A	124	$C_{10}H_{22}$ isomer
36	125	styrene
37	126	*o*-xylene
37A	127	C_9H_{18} isomer
38	129	*n*-nonane
38A	131	$C_{10}H_{20}$ isomer
39	132	$C_{10}H_{22}$ isomer + isopropylbenzene
39A	134	$C_{10}H_{20}$ isomer
40	135	$C_{10}H_{22}$ isomer + propylcyclohexane
40A	136	unsat. hydrocarbon
41	139	*n*-propylbenzene
42	140	benzaldehyde
42A	141	ethyltoluene isomer
43	142	$C_{11}H_{24}$ isomer
44	144	$C_{11}H_{24}$ isomer
45	147	C_3-alkyl benzene isomer
46	148	*n*-decane
47	149	C_4-alkyl benzene isomer
47A	150	C_4-alkyl benzene isomer
47B	151	$C_{11}H_{24}$ isomer
48	152	1,2,3-trimethylbenzene + $C_{11}H_{24}$ isomer
48A	152	$C_{12}H_{26}$ isomer
49	153	$C_{11}H_{24}$ isomer
50	156	C_4-alkyl benzene isomer
51	157	C_4-alkyl benzene isomer
51A	158	$C_{11}H_{24}$ isomer
52	160	acetophenone
52A	162	C_4-alkyl benzene isomer
52B	163	$C_{11}H_{22}$ isomer
53	166	*n*-undecane
54	175	sat. hydrocarbon
54A	177	$C_{12}H_{26}$ isomer
55	181	$C_{12}H_{24}$ isomer
55A	182	naphthalene
56	183	*n*-dodecane
56A	184	$C_{12}H_{24}$ isomer
57	185	sat. hydrocarbon (tent.)
58	186	$C_{13}H_{28}$ isomer
59	192	unsat. hydrocarbon
60	198	*n*-tridecane
62	212	*n*-tetradecane

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[a] See Table 42 for protocol.

Table A4. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM BATON ROUGE, LA AREA (P5/L2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	41	$N_2 + O_2$
2	42	CO_2
2A	43	xenon (traces)
3	46	propane
3A	47	C_4H_8 isomer + vinyl chloride (traces)(tent.)
4	48	*n*-butane
4A	49	C_4H_8 isomer
5	50	acetaldehyde
5A	51	ethyl chloride (traces)
6	52	C_5H_{10} isomer
7	53	isopentane
8A	55	propanal
9	56	acetone + *n*-pentane
10	57	C_5H_{10} isomer
10A	57	$C_4H_{10}O$ isomer (tent.)
11	57	dichloroethylene isomer (tent.)
11A	58	C_5H_{10} isomer
12	58	methylene chloride
14	60	cyclopentadiene
14A	62	cyclopentene
15	63	C_6H_{12} isomer
15A	64	cyclopentane
16	65	2-methylpentane
17	66	1,5-hexadiene
18	67	3-methylpentane
19	68	2-methyl-1-pentene
19A	69	hexafluorobenzene (e[illegible])
20	70	*n*-hexane
21	71	C_6H_{12} isomer
21A	71	methyl ethyl ketone
22	72	C_6H_{12} + C_6H_{10} isomers
23	73	ethyl acetate
23A	74	perfluorotoluene (e[illegible])
24	75	methylcyclopentane
25	76	1,2-dichloroethane
26	77	1,1,1-trichloroethane
26A	78	C_6H_8 isomer
26B	79	C_6H_{10} isomer
27	80	benzene
27A	81	carbon tetrachloride
28	81	cyclohexane
29	82	2-methylhexane
29A	83	2,3-dimethylpentane
30	84	3-methylhexane
30A	84	C_6H_{10} isomer
31	86	C_7H_{14} isomer
32	87	trichloroethylene + *n*-pentanal
32A	88	C_7H_{14} isomer
33	89	*n*-heptane
33A	89	C_7H_{12} isomer
33B	90	C_7H_{14} isomer
33C	91	C_7H_{14} isomer
34	91	diisobutylene
34A	92	C_7H_{14} isomer
34B	93	C_7H_{12} isomer
35	96	methylcyclohexane
36	95	C_8H_{18} isomer
37	96	4-methyl-2-pentanone + C_8H_{18} isomer
38	98	C_8H_{16} isomer
39	100	1,1,2-trichloroethane
39A	100	C_8H_{14} isomer
40	101	toluene
41	102	C_8H_{18} isomer
42	104	C_8H_{18} isomer
43	105	C_8H_{16} isomer
44	106	C_9H_{20} isomer
44A	107	C_8H_{16} isomer
45	108	C_8H_{16} isomer
45A	108	1,2-dibromoethane
45B	109	C_8H_{16} isomer
46	109	*n*-octane
46A	110	C_8H_{16} isomer
47	111	tetrachloroethylene
48	112	C_9H_{18} isomer
48A	112	C_9H_{18} isomer
49	113	C_9H_{20} isomer
50	114	C_9H_{20} isomer
50A	114	C_9H_{18} isomer
51	115	C_9H_{20} isomer
52	116	C_9H_{18} isomer
53	117	C_9H_{20} isomer + 1,1,1,2-tetrachloroethane (traces)
53A	118	C_9H_{18} isomer
54	118	C_9H_{18} isomer
55	119	C_9H_{18} isomer
56	120	ethylbenzene
57	121	C_9H_{18} isomer
58	122	*m*- and/or *p*-xylene
58A	122	C_9H_{20} isomer
58B	123	C_9H_{18} isomer
59	124	C_9H_{20} isomer

(continued)

Table A4 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
59A	125	C_9H_{18} isomer
59B	125	$C_{10}H_{22}$ isomer
60	126	styrene
60A	126	C_9H_{18} isomer
61	127	*o*-xylene
61A	128	C_9H_{18} isomer
62	129	*n*-nonane
62A	130	C_9H_{18} isomer
63	132	C_9H_{12} isomer
63A	132	$C_{10}H_{20}$ isomer
64	133	isopropylbenzene + $C_{10}H_{22}$ isomer
65	134	$C_{10}H_{22}$ isomer
65A	135	$C_{10}H_{20}$ isomer
65B	136	propylcyclohexane
66	136	$C_{10}H_{22}$ isomer
67	138	$C_{10}H_{20}$ isomer
68	139	*n*-propylbenzene
69	140	*m*- and/or *p*-ethyltoluene
70	141	$C_{10}H_{22}$ isomer
71	142	1,3,5-trimethylbenzene
71A	142	$C_{11}H_{24}$ isomer
72	143	$C_{10}H_{22}$ isomer
73	144	*o*-ethyltoluene
74	144	$C_{11}H_{24}$ isomer
74A	145	$C_{10}H_{20}$ isomer
75	145	$C_{11}H_{24}$ isomer
75A	146	$C_{10}H_{20}$ + C_9H_{10} isomers
76	146	1,2,4-trimethylbenzene
76A	147	$C_{10}H_{20}$ isomer
77	148	*n*-decane
78	149	triisobutylene
78A	149	$C_{11}H_{22}$ isomer
78B	150	C_4-alkyl benzene isomer
79	151	$C_{11}H_{24}$ isomer
79A	151	C_4-alkyl benzene isomer
80	152	1,2,3-trimethylbenzene
81	152	$C_{11}H_{24}$ isomer
82	153	$C_{11}H_{24}$ isomer
82A	153	$C_{10}H_{12}$ isomer
82B	154	indan
83	155	butylcyclohexane + $C_{11}H_{24}$ isomer
83A	155	$C_{11}H_{22}$ isomer
84	156	$C_{12}H_{26}$ + C_4-alkyl benzene isomers
84A	157	C_4-alkyl benzene + $C_{11}H_{22}$ isomers
85	158	C_4-alkyl benzene isomer
86	158	$C_{11}H_{24}$ isomer
87	159	$C_{11}H_{22}$ isomer
87A	159	$C_{11}H_{24}$ isomer
88	160	acetophenone
88A	160	$C_{10}H_{18}$ isomer
89	161	$C_{11}H_{24}$ isomer
90	162	C_4-alkyl benzene isomer
90A	162	$C_{11}H_{22}$ isomer
90B	103	C_4H_7 benzene isomer
91	163	C_4- alkyl benzene isomer
92	168	$C_{11}H_{22}$ isomer
93	166	*n*-undecane
93A	168	$C_{12}H_{26}$ isomer
93B	168	C_4- alkyl benzene isomer
94	169	$C_{12}H_{26}$ isomer
94A	169	C_4-alkyl benzene isomer
95	170	$C_{12}H_{26}$ isomer
95A	171	$C_{12}H_{24}$ isomer
95B	171	C_5-alkyl benzene isomer
95C	172	C_5-alkyl benzene isomer
96	173	$C_{11}H_{22}$ isomer
96A	173	$C_{12}H_{24}$ isomer
96B	174	C_5-alkyl benzene isomer
97	175	$C_{12}H_{26}$ + C_4 alkyl benzene isomers
98	175	C_5-alkyl benzene + $C_{12}H_{26}$ isomers
99	176	$C_{12}H_{26}$ isomer
99A	176	C_5- alkyl benzene isomer
100	177	$C_{12}H_{26}$ isomer
100A	177	C_5- alkyl benzene isomer
100B	179	unsat. hydrocarbon
100C	180	$C_{13}H_{24}$ isomer
101	180	naphthalene
102	183	*n*-dodecane
103	184	$C_{13}H_{28}$ isomer
104	186	1,3-hexachlorobutadiene
104A	189	C_6-alkyl cyclohexane isomer
104B	190	$C_{13}H_{28}$ isomer
104C	191	$C_{13}H_{28}$ isomer
105	193	$C_{13}H_{28}$ isomer
105A	193	$C_{13}H_{26}$ isomer
105B	195	$C_{13}H_{26}$ isomer
106	197	*n*-tridecane
106A	198	β-methylnaphthalene
106B	199	$C_{15}H_{32}$ isomer
106C	200	α-methylnaphthalene
106D	205	$C_{15}H_{30}$ isomer
106E	206	$C_{14}H_{30}$ isomer
106F	210	$C_{14}H_{28}$ isomer
107	211	*n*-tetradecane

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[a] See Table 42 for protocol.

Table A5. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM BATON ROUGE, LA AREA (P5/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2
2A	45	propane
2B	46	C_4H_8 isomer
2C	46	C_4H_{10} isomer
3	48	acetaldehyde
4	50	isopentane
5A	51	C_5H_{10} isomer
5B	51	C_5H_8 isomer
5C	51	n-pentane
6	52	acetone
6A	52	C_5H_{10} isomer
7	53	methylene chloride + C_5H_8 isomer
9	55	cyclopentadiene
9A	55	t-butanol
9B	56	cyclopentene
10	57	C_6H_{12} isomer
10A	58	cyclopentane
11	58	2-methylpentane
12	59	1,5-hexadiene
13	60	3-methylpentane
14	61	2-methyl-1-pentene
14A	62	hexafluorobenzene (eM)
15	62	n-hexane
15A	63	diisopropyl ether
15B	63	C_6H_{12} isomer
15C	64	C_6H_{10} isomer
16	65	C_6H_{12} isomer
16A	66	perfluorotoluene (eM)
17	68	methylcyclopentane
18	70	1,1,1-trichloroethane
19	73	benzene
19A	74	cyclohexane
20	75	2-methylhexane
21	77	3-methylhexane
21A	78	cyclohexane or C_6H_{10} isomer
21B	79	C_7H_{14} isomer
22	80	C_8H_{18} isomer
22A	80	trichloroethylene
23	82	n-heptane
24	85	C_8H_{16} isomer
24A	87	C_7H_{12} isomer
25	88	methylcyclohexane
26	90	C_8H_{18} isomer
26A	91	C_8H_{16} isomer
27	92	4-methyl-2-pentanone
27A	92	C_8H_{16} isomer
28	94	C_8H_{16} isomer
28A	95	C_7H_{12} isomer
29	96	toluene
30	97	C_8H_{18} isomer
31	99	C_8H_{18} isomer
32	100	C_8H_{16} isomer
33	102	C_8H_{16} isomer
33A	103	C_8H_{16} isomer
34	105	n-octane
34A	105	C_8H_{16} isomer
35	106	tetrachloroethylene
35A	108	C_9H_{18} isomer
36	109	C_9H_{20} isomer
37	110	C_9H_{20} isomer
37A	110	C_9H_{18} isomer
38	112	4-vinyl-1-cyclohexane
38A	112	C_9H_{18} isomer
39	113	C_9H_{20} isomer
39A	114	C_9H_{18} isomer
40	115	C_9H_{18} isomer
41	117	ethylbenzene
41A	118	C_9H_{18} isomer
42	119	m- and/or p-xylene
43	121	C_9H_{20} isomer
44	122	C_9H_{18} isomer
45	123	styrene
46	125	o-xylene
46A	126	C_9H_{18} isomer
47	127	n-nonane
47A	129	C_9H_{18} isomer
48	130	C_9H_{12} isomer
49	131	isopropylbenzene
50	132	$C_{10}H_{22}$ isomer
51	133	$C_{10}H_{22}$ isomer
51A	133	$C_{10}H_{20}$ isomer
51B	133	propylcyclohexane
52	134	$C_{10}H_{22}$ isomer
53	136	$C_{10}H_{20}$ isomer
53A	136	$C_{11}H_{24}$ isomer
54	137	n-propylbenzene
54A	137	benzaldehyde
55	138	ethyltoluene isomer
55A	139	$C_{10}H_{20}$ isomer
56	140	1,3,5-trimethylbenzene + $C_{11}H_{24}$ isomer

(continued)

Table A5 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
56A	140	$C_{10}H_{20}$ isomer
57	141	$C_{10}H_{22}$ isomer
58	142	C_3H_5-benzene isomer + *o*-ethyl benzene
58A	142	$C_{10}H_{18}$ + $C_{10}H_{20}$ isomers
58B	143	$C_{11}H_{24}$ isomer
59	144	1-methyl-4-isopropylcyclohexane
59A	144	C_3H_5-benzene isomer
60	145	1,2,4-trimethylbenzene
60A	146	$C_{10}H_{20}$ isomer
61	147	*n*-decane
61A	147	$C_{10}H_{20}$ isomer
62	148	triisobutylene + C_4-alkyl benzene isomer
62A	149	C_4-alkyl benzene isomer
63	150	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
64	151	C_4-alkyl benzene isomer
65	152	$C_{11}H_{24}$ isomer
66	153	$C_{11}H_{24}$ isomer
66A	153	indan
67	154	C_4-alkyl cyclohexane isomer
67A	155	indene (traces) + $C_{11}H_{22}$ isomer
68	156	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
68A	156	C_4-alkyl benzene isomer
69	157	C_4-alkyl benzene isomer
70	158	$C_{11}H_{24}$ isomer
71	158	$C_{11}H_{24}$ isomer
72	159	acetophenone + $C_{11}H_{24}$ isomer
73	160	$C_{11}H_{24}$ isomer
74	161	C_4-alkyl benzene isomer
74A	161	$C_{11}H_{22}$ isomer
74B	162	C_4H_7 benzene isomer (traces)
75	162	C_4-alkyl benzene isomer
76	164	$C_{11}H_{22}$ isomer
76A	164	C_4H_7 benzene isomer
77	165	*n*-undecane
77A	166	$C_{11}H_{22}$ isomer
77B	166	C_4-alkyl benzene isomer
77C	167	$C_{11}H_{22}$ isomer
77D	168	$C_{12}H_{26}$ isomer
78	169	C_4-alkyl benzene isomer
78A	170	$C_{11}H_{20}$ isomer
79	170	$C_{12}H_{26}$ isomer
79A	171	$C_{12}H_{24}$ isomer
80	172	C_5-alkyl benzene isomer
81	173	unsat. hydrocarbon
81A	174	C_5-alkyl benzene isomer
81B	174	C_4H_7 benzene isomer
82	175	C_4-alkyl benzene isomer
83	175	C_5-alkyl benzene isomer
84	176	$C_{12}H_{26}$ isomer
84A	176	C_5-alkyl benzene isomer
84B	177	$C_{12}H_{26}$ isomer
85	177	C_5-alkyl benzene isomer
85A	179	unsat. hydrocarbon
86	180	naphthalene
86A	181	C_5-alkyl benzene isomer
87	182	*n*-dodecane
87A	183	$C_{12}H_{24}$ isomer
87B	183	C_5-alkyl benzene isomer
88	184	$C_{13}H_{28}$ isomer
89	185	$C_{13}H_{26}$ isomer
89A	189	C_6-alkyl cyclohexane isomer
90	191	1-phenylhexane
91	194	$C_{14}H_{30}$ isomer
91A	196	unsat. hydrocarbon
92	197	*n*-tridecane
93	199	β-methylnaphthalene
93A	201	α-methylnaphthalene
93B	204	unsat. hydrocarbon
94	205	unsat. hydrocarbon
94A	207	C_7-alkyl benzene isomer
95	209	$C_{15}H_{32}$ isomer
96	212	$C_{14}H_{30}$ isomer
96A	213	C_2-alkyl naphthalene isomer
96B	217	unsat. hydrocarbon
96C	218	sat. hydrocarbon

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[a] See Table 42 for protocol.

Table A6. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM BATON ROUGE, LA AREA (P6/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2	39A	113	ethylcyclohexane
2A	46	C_4H_8 isomer	40	113	C_9H_{20} isomer
3	47	acetaldehyde	40A	114	C_9H_{18} isomer
3A	47A	isopentane	41	117	ethylbenzene
5	52	n-pentane	41A	117	trichloropropene
6	53	acetone	42	119	m- and/or p-xylene
7	54	vinylidene chloride	43	121	C_9H_{20} isomer
7A	54A	methylene chloride	44	123	styrene
9	55	dichloroethylene isomer	45	124	o-xylene
9A	55A	cyclopentane	45A	125	1,1,2,2-tetrachloroethane
10	60	2-methylpentane	45B	126	C_9H_{18} isomer
11	62	3-methylpentane	46	127	n-nonane
12	63	hexafluorobenzene (eS)	46A	129	trichloropropene isomer (tent.)
13	64	n-hexane	47	131	$C_{10}H_{22}$ isomer + isopropylbenzene
14	65	chloroform	48	132	$C_{10}H_{22}$ isomer
15	67	ethyl acetate	49	134	$C_{10}H_{22}$ isomer
16	68	perfluorotoluene (eS)	49A	135	$C_{10}H_{22}$ isomer
16A	68A	methylcyclopentane	50	137	n-propylbenzene
17	70	1,2-dichloroethane	51	138	m- and/or p-ethyltoluene
18	71	1,1,1-trichloroethane	52	139	$C_{10}H_{22}$ isomer
18A	71A	C_7H_{16} isomer	53	140	1,3,5-trimethylbenzene + $C_{11}H_{24}$ isomer
19	74	benzene	53A	140	pentachloroethane
20	75	carbon tetrachloride	53B	141	benzaldehyde
20A	75A	cyclohexane	54	141	$C_{10}H_{22}$ isomer
21	76	2-methylhexane	55	142	o-ethyltoluene
21A	76A	C_7H_{14} isomer	56	143	$C_{11}H_{24}$ isomer
22	78	3-methylhexane	56A	144	C_3H_5 benzene isomer
23	80	1,2-dichloropropane	57	145	1,2,4-trimethylbenzene
24	81	trichloroethylene	58	147	n-decane
25	83	n-heptane	58A	147	C_3H_5-benzene isomer
25A	83A	C_8H_{18} isomer (tent)	59	148	C_4-alkyl benzene isomer
26	89	methylcyclohexane	59A	149	$C_{10}H_{20}$ isomer
27	91	C_8H_{18} isomer	59B	149	$C_{11}H_{22}$ isomer
28	92	4-methyl-2-pentanone	59C	150	C_4-alkyl benzene isomer
29	93	C_8H_{16} isomer (tent)	60	151	1,2,3-trimethylbenzene + $C_{11}H_{24}$ isomer
30	95	1,1,2-trichloroethane	61	152	$C_{11}H_{24}$ isomer
31	97	toluene	61A	153	indan
32	98	C_8H_{18} isomer	62	154	$C_{11}H_{24}$ isomer
33	100	C_8H_{18} isomer	63	155	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
34	101	C_8H_{16} isomer	63A	156	C_4-alkyl benzene isomer
34A	101A	C_8H_{16} isomer	64	157	C_4-alkyl benzene isomer
35	105	n-octane	64A	157	$C_{11}H_{24}$ isomer
36	107	tetrachloroethylene	64B	158	$C_{11}H_{24}$ isomer
37	109	C_9H_{20} isomer	65	159	C_4-alkyl benzene isomer
38	111	C_9H_{20} isomer	65A	159	acetophenone
39	112	C_9H_{20} isomer	65B	160	$C_{11}H_{24}$ isomer

(continued)

Table A6 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
65C	160	C_4-alkyl benzene isomer
66	161	hexachloroethane isomer
67	162	C_4-alkyl benzene isomer
68	165	n-undecane
68A	166	C_4-alkyl benzene isomer
69	168	C_4-alkyl benzene isomer
69A	170	C_5-alkyl benzene isomer
70	172	$C_{11}H_{22}$ isomer
70A	172	C_5-alkyl benzene isomer
71	174	$C_{12}H_{26}$ isomer
71A	175	C_4-alkyl benzene isomer
71B	175	C_5-alkyl benzene isomer
72	176	$C_{12}H_{26}$ isomer
72A	178	C_5-alkyl benzene isomer
72B	180	C_5-alkyl benzene isomer
73	180	naphthalene
74	181	n-dodecane
75	185	1,3-hexachlorobutadiene
75A	189	unsat. hydrocarbon
75B	193	$C_{14}H_{30}$ isomer
75C	194	$C_{13}H_{26}$ isomer
76	197	n-tridecane
76A	199	β-methylnaphthalene
76B	201	α-methylnaphthalene
76C	211	sat. hydrocarbon

[a] See Table 42 for protocol.

Part II - LAKE CHARLES, LA

Table A7. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P1/L1 - B/T_2)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	84	benzene	3	189	dibromocyclohexane isomer
2	104	toluene			

[a] See Table 43 and 6 for protocol and experimental design.

Table A8. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P1/L1 - A/T_1)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	67	hexafluorobenzene (eI)	6A	79	carbon tetrachloride (traces)
2	69	chloroform	7	86	trichloroethylene
3	72	perfluorotoluene (eI)	8	101	toluene
4	74	1,2-dichloroethane	9	115	tetrachloroethylene
5	75	1,1,1-trichloroethane	9A	158	dichlorobenzene isomer (traces)
6	78	benzene			

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A9. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P3/L1 - A/T_2)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2	8	80	benzene
2	58	methylene chloride	9	81	carbon tetrachloride (traces)
3	69	hexafluorobenzene (eS)	10	88	trichloroethylene (traces)
4	71	chloroform	11	103	toluene
5	74	perfluorotoluene (eS)	12	113	tetrachloroethylene
6	76	1,2-dichloroethane	13	126	bromoform
7	77	1,1,1-trichloroethane	14	193	dibromocyclohexane isomer

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A10. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P3/L1 - B2/T_2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2	9	78	benzene
2	47	chloromethane (traces)	10	79	carbon tetrachloride (traces)
3	58	methylene chloride (traces)	11	85	chloromethylbutene isomer
4	67	hexafluorobenzene (eS)	12	87	trichloroethylene
5	69	chloroform	13	101	toluene
6	73	perfluorotoluene (eS)	14	111	tetrachloroethylene
7	74	1,2-dichloroethane	15	151	dichlorobenzene isomer (trace)
8	75	1,1,1-trichloroethane			

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A11. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P3/L1 - B2/T_2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
2	56	methylene chloride (traces)
3	67	hexafluorobenzene (eS)
4	69	chloroform
5	72	perfluorotoluene (eS)
6	74	1,2-dichloroethane
7	75	1,1,1-trichloroethane
8	78	benzene
9	79	carbon tetrachloride (traces)
10	86	trichloroethylene (traces)
11	100	toluene
12	111	tetrachloroethylene
13	124	bromoform (traces)
14	191	dibromocyclohexane isomer

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A12. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P4/L1 - B1/T_2)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	47	chloromethane (traces)
2	57	vinylidene chloride
3	58	methylene chloride (traces)
4	68	hexafluorobenzene (eS)
5	70	chloroform
6	73	perfluorotoluene (eS)
7	75	1,2-dichloroethane
8	76	1,1,1-trichloroethane
9	80	carbon tetrachloride
10	88	trichloroethylene
11	111	tetrachloroethylene
12	151	dichlorobenzene isomer (trace)

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A13. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P4/L1 - B/T_2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2	56	vinylidene chloride
3	66	hexafluorobenzene (eS)
4	68	chloroform
5	71	perfluorotoluene (eS)
6	73	1,2-dichloroethane
7	74	1,1,1-trichloroethane
8	78	carbon tetrachloride
9	84	trichloroethylene
10	110	tetrachloroethylene
11	190	dibromocyclohexane isomer

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A14. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA ($P4/L1 - A2/T_3$)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	69	chloroform	5	86	trichloroethylene
2	75	1,2-dichloroethane	6	111	tetrachloroethylene
3	76	1,1,1-trichloroethane	7	124	bromoform
4	80	carbon tetrachloride (traces)	8	190	dibromocyclohexane isomer

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A15. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P5/L1 - B2/T_2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	57	methylene chloride	8	86	trichloroethylene
2	67	hexafluorobenzene (eS)	9	99	1,1,2-trichloroethane
3	69	chloroform	10	111	tetrachloroethylene
4	72	perfluorotoluene (eS)	11	125	bromoform
5	74	1,2-dichloroethane	12	151	dichlorobenzene isomer (tent.)
6	75	1,1,1-trichloroethane	13	191	dibromocyclohexane isomer

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A16. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P5/L1 - A/T_3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	58	dichloromethane
2	67	hexafluorobenzene (eS)
3	69	chloroform
4	73	perfluorotoluene (eS)
5	74	1,2-dichloroethane
6	75	1,1,1-trichloroethane
7	78	carbon tetrachloride
8	86	trichloroethylene
9	100	1,1,2-trichloroethane
10	111	tetrachloroethylene
11	125	bromoform
12	189	dibromocyclohexane isomer

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A17. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P5/L1 - B1/T_2)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	57	methylene chloride	7	78	carbon tetrachloride
2	66	hexafluorobenzene (eS)	8	85	trichloroethylene
3	68	chloroform	9	98	1,1,2-trichloroethane
4	71	perfluorotoluene (eS)	10	110	tetrachloroethylene
5	73	1,2-dichloroethane	11	139	2,3-dichloro-1-propanol (tent.)
6	74	1,1,1-trichloroethane	12	151	dichlorobenzene isomer (trace)

[a] See Tables 43 and 6 for sampling protocol and experimental design.

Table A18. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P7/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
1A	44	xenon (traces)
2	45	CF_2Cl_2
3	47	vinyl chloride
3A	47	C_4H_8 isomer
4	48	C_4H_{10} isomer
4A	48	acetaldehyde
5	50	ethyl chloride
5A	53	isopentane
6	53	$CFCL_3$
7	55	n-pentane
7A	56	acetone
8	56	vinylidene chloride
9	57	methylene chloride
10	58	Freon 113
10A	60	alcohol (tent.)
11	61	dichloroethylene isomer
11A	62	C_5H_{10} isomer
12	63	2-methylpentane
13	65	3-methylpentane
13A	66	C_6H_{12} isomer
14	66	hexafluorobenzene (eS)
15	67	dichloroethylene isomer
16	68	n-hexane
16A	68	methyl ethyl ketone
17	69	chloroform
18	70	ethyl acetate
19	72	perfluorotoluene (eS)
19A	72	methylcyclopentane
20	73	1,2-dichloroethane
21	75	1,1,1-trichloroethane
22	78	benzene
22A	78	carbon tetrachloride
22B	79	cyclohexane
23	80	2-methylhexane
24	82	3-methylhexane
24A	83	$C_5H_{10}0$ isomer (tent.)
25	84	C_7H_{14} isomer
26	85	trichloroethylene
27	87	n-heptane
27A	88	acetic acid (tent.)
27B	89	C_7H_{14} isomer
28	92	methylcyclohexane
28A	93	C_8H_{18} isomer
29	94	C_8H_{18} isomer
30	97	C_8H_{16} isomer
31	98	1,1,2-trichloroethane
32	100	toluene
33	102	C_8H_{18} isomer
84	104	C_8H_{18} isomer
35	105	C_8H_{16} isomer
36	105	C_8H_{18} isomer
37	106	C_8H_{16} isomer
37A	107	C_8H_{16} isomer
38	109	n-octane
39	110	tetrachloroethylene
40	114	C_9H_{20} isomer
41	116	C_9H_{20} isomer
41A	116	C_9H_{18} isomer
42	117	1,1,1,2-tetrachloroethane
42A	117	C_9H_{20} isomer
43	118	chlorobenzene
43A	119	C_9H_{18} isomer
43B	120	C_9H_{18} isomer
44	121	ethylbenzene
45	123	m- and/or p-xylene
45A	121	C_9H_{20} isomer
46	125	C_9H_{20} isomer
47	126	C_9H_{20} isomer
47A	127	styrene + heptanal (tent.)
47B	127	o-xylene
48	128	1,1,2,2-tetrachloroethane
48A	129	C_9H_{18} isomer
49	130	n-nonane
49A	132	C_9H_{18} isomer
49B	133	C_9H_{18} isomer
49C	133	$C_{10}H_{22}$ isomer
50	134	$C_{10}H_{22}$ isomer
50A	135	isopropylbenzene
51	136	$C_{10}H_{22}$ isomer
51A	137	C_3-alkyl cyclohexane isomer
52	138	$C_{10}H_{22}$ isomer
52A	139	$C_{10}H_{22}$ isomer
52B	140	$C_{10}H_{20}$ isomer
53	141	n-propylbenzene
54	142	m- and/or p-ethyltoluene
54A	143	$C_{10}H_{22}$ isomer
54B	143	1,3,5-trimethylbenzene
55	144	$C_{11}H_{24}$ isomer + pentachloroethane
56	145	$C_{10}H_{22}$ isomer

(continued)

Table A18 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
56A	145	benzaldehyde
56B	145	o-ethyltoluene
57	146	$C_{11}H_{24}$ isomer
57A	147	$C_{10}H_{20}$ isomer
57B	148	$C_{10}H_{20}$ isomer
58	148	1,2,4-trimethylbenzene
58A	149	$C_{10}H_{20}$ isomer
59	150	n-decane
59A	151	C_4-alkyl benzene isomer
60	152	dichlorobenzene isomer
60A	152	$C_{11}H_{24}$ isomer
60B	152	$C_{11}H_{22}$ isomer
61	153	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
62	154	1,2,3-trimethylbenzene
62A	155	C_4-alkyl benzene isomer
63	156	$C_{11}H_{24}$ isomer
63A	156	dichlorobenzene isomer
63B	157	indan
64	157	C_4 alkyl cyclohexane isomer
65	158	$C_{11}H_{24}$ isomer
65A	159	C_4-alkyl benzene isomer
66	160	C_4-alkyl benzene isomer
66A	161	$C_{11}H_{24}$ isomer
67	162	$C_{11}H_{24}$ isomer
67A	162	C_4-alkyl benzene isomer
68	163	acetophenone
68A	164	C_4-alkyl benzene isomer
68B	164	pentachlorobromoethane (tent.)
68C	165	C_4H_7-benzene isomer
69	165	C_4-alkyl benzene isomer
69A	166	C_4H_7-benzene isomer
70	157	$C_{11}H_{22}$ isomer
71	168	n-undecane
72	169	$C_{11}H_{24}$ isomer
73	171	C_4-alkyl benzene + $C_{12}H_{26}$ isomers
74	173	$C_{11}H_{20}$ isomer
74A	173	$C_{12}H_{26}$ isomer
74B	174	C_5-alkyl benzene isomer
74C	175	$C_{12}H_{24}$ isomer
75	175	C_6-alkyl cyclohexane isomer
75A	176	$C_{11}H_{20}$ isomer
76	177	$C_{12}H_{26}$ isomer
76A	177	C_5 alkyl benzene isomer
77	179	$C_{12}H_{26}$ isomer
77A	180	pentachlorobutadiene
77B	181	$C_{12}H_{26}$ isomer
77C	182	$C_{12}H_{24}$ isomer
78	183	naphthalene
79	184	n-dodecane
79A	186	$C_{12}H_{24}$ isomer
80	187	$C_{13}H_{28}$ isomer
81	189	hexachlorobutadiene
81A	191	$C_{12}H_{24}$ isomer
82	192	$C_{13}H_{28}$ isomer
83	196	$C_{14}H_{30}$ isomer
84	200	n-tridecane
84A	202	β-methylnaphthalene
84B	203	$C_{14}H_{30}$ isomer
84C	204	α-methylnaphthalene
85	212	$C_{14}H_{30}$ isomer
85A	214	biphenyl
86	215	n-tetradecane
86A	216	diphenyl ether
87	228	$C_{15}H_{32}$ isomer
88	240	2,2,4-trimethylpenta-1,3-diol di-isobutyrate (BKG)

[a] See Table 43 for sampling protocol.

Table A19. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM LAKE CHARLES, LA (P8/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2
1A		xenon (traces)
3	46	isobutane
3A		C_4H_8 isomer
3B		acetaldehyde
4	47	n-butane
6	52	isopentane
7	53	n-pentane
7A	55	C_5H_{10} isomer
8	56	methylene chloride
9	57	acetone
9A	57	alcohol (tent.)
10	61	cyclopentane
10A	61	2-methylpentane
11	64	3-methylpentane
11A	64	C_6H_{12} isomer
12	65	hexafluorobenzene (eS)
13	66	n-hexane
13A	67	chloroform
14	69	ethyl acetate
15	70	perfluorotoluene (eS)
15A	71	methylcyclopentane
15B	72	1,2-dichloroethane
15C	73	1,1,1-trichloroethane
15D	76	C_6H_{10} isomer
16	77	benzene
16A	77	carbon tetrachloride
16B	78	cyclohexane
17	79	2-methylhexane
17A	80	2,3-dimethylpentane
18	81	3-methylhexane
18A	83	C_7H_{14} isomer
19	83	C_7H_{14} isomer
20	84	C_8H_{18} isomer
20A	85	trichloroethylene
20B	86	pentanal
21	86	n-heptane
21A	87	C_7H_{14} isomer
21B	91	C_8H_{18} isomer
22	92	methylcyclohexane
22A	94	C_8H_{18} isomer
23	94	C_8H_{18} isomer
24	96	C_8H_{16} isomer
24A	97	C_8H_{16} isomer
25	98	C_8H_{18} isomer
26	99	toluene
27	101	C_8H_{18} isomer
28	102	C_8H_{18} isomer
29	104	dimethylcyclohexane
30	105	C_9H_{20} isomer
31	106	C_8H_{16} isomer
31A	107	C_8H_{16} isomer
32	108	n-octane
32A	109	C_8H_{16} isomer
33	110	tetrachloroethylene
33A	110	C_8H_{16} isomer
34	112	C_9H_{20} isomer
35	114	C_9H_{20} isomer
35A	115	C_9H_{18} isomer
36	115	C_9H_{20} isomer
36A	116	C_9H_{18} isomer
37	117	ethylcyclohexane + C_9H_{20} isomer
37A	118	C_9H_{18} isomer
37B	120	$C_6H_{12}O$ isomer (tent.)
38	121	ethylbenzene
38A	122	C_9H_{18} isomer
39	123	m- and/or p-xylene
40	124	C_9H_{20} isomer
41	126	C_9H_{20} isomer
41A	127	C_9H_{18} isomer
41B	128	styrene
42	128	o-xylene + C_9H_{20} isomer
42A	129	C_9H_{18} isomer
43	130	n-nonane
43A	131	$C_{10}H_{22}$ isomer
43B	132	C_9H_{18} isomer
44	133	C_9H_{18} isomer
45	134	$C_{10}H_{22}$ isomer
45A	135	isopropylbenzene
45B	136	C_9H_{16} isomer
46	136	$C_{10}H_{22}$ isomer
46A	137	$C_{10}H_{20}$ isomer
47	138	propylcyclohexane + $C_{10}H_{22}$ isomer
47A	138	$C_{10}H_{20}$ isomer
47B	139	$C_{10}H_{16}$ isomer
47C	140	$C_{10}H_{20}$ isomer
48	141	n-propylbenzene
49	142	m- and/or p-ethyltoluene
49A	143	$C_{10}H_{22}$ isomer
49B	144	1,3,5-trimethylbenzene

(continued)

Table A19 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
50	144	$C_{11}H_{24}$ isomer
51	145	benzaldehyde
51A	145	$C_{10}H_{22}$ isomer
52	146	*o*-ethyltoluene + $C_{11}H_{24}$ isomer
53	147	$C_{11}H_{24}$ isomer
53A	149	$C_{10}H_{20}$ isomer
54	149	1,2,4-trimethylbenzene
54A	150	$C_{10}H_{20}$ isomer
55	151	*n*-decane
55A	152	$C_{10}H_{20}$ isomer
56	152	$C_{11}H_{24}$ isomer
56A	152	C_4-alkyl benzene isomer
56B	153	dichlorobenzene isomer
56C	154	$C_{11}H_{24}$ isomer
57	154	1,2,3-trimethylbenzene
57A	155	$C_{11}H_{24}$ isomer
58	156	$C_{12}H_{26}$ isomer
58A	157	indan
59	157	$C_{12}H_{26}$ isomer
59A	158	$C_{10}H_{20}$ isomer
60	159	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
60A	159	C_4-alkyl benzene isomer
61	161	C_4-alkyl benzene isomer
61A	161	$C_{11}H_{24}$ isomer
61B	162	$C_{11}H_{22}$ isomer
61C	162	$C_{11}H_{24}$ isomer
62	163	$C_{11}H_{24}$ isomer
62A	163	C_4-alkyl benzene isomer
62B	163	$C_{10}H_{18}$ isomer
62B	163	$C_{10}H_{18}$ isomer
62C	164	acetophenone
62D	164	C_4-alkyl benzene isomer
62E	165	$C_{11}H_{22}$ isomer
62F	166	C_4H_7-benzene isomer
63	166	C_4-alkyl benzene isomer
63A	167	C_4H_7-benzene isomer
63B	167	$C_{11}H_{22}$ isomer
64	168	*n*-undecane
64A	169	C_4-alkyl benzene isomer
65	172	C_4-alkyl benzene isomer
65A	175	C_5-alkyl benzene isomer
65B	176	C_5-alkyl benzene isomer
65C	176	C_4H_7-benzene isomer
65D	177	$C_{12}H_{24}$ isomer
65E	177	C_5-alkyl benzene isomer
66	178	$C_{12}H_{26}$ isomer
66A	178	C_5-alkyl benzene isomer
66B	179	$C_{12}H_{26}$ isomer
66C	180	$C_{12}H_{26}$ isomer
66D	180	C_5-alkyl benzene isomer
66E	184	naphthalene
67	185	*n*-dodecane
67A	192	$C_{12}H_{24}$ isomer
67B	195	$C_{13}H_{26}$ isomer
68	200	*n*-tridecane
68A	202	β-methylnaphthalene
68B	204	α-methylnaphthalene
69	217	*n*-tetradecane

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[a] See Table 43 for sampling protocol.

Part III - BEAUMONT, TX

Table A20. VAPOR-PHASE HALOGENATED AND OTHER SELECTED ORGANICS IN AMBIENT AIR FROM BEAUMONT, TX (P2/L2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2
1A	43	xenon
2A	45	chloromethane (traces) (tent.)
3	46	isobutane
3A	47	C_4H_8 isomer
4	48	acetaldehyde
4A	49	n-butane
4B	50	C_4H_8 isomer
6	54	isopentane
7A	56	n-pentane
8	57	acetone
9	59	methylene chloride
10A	62	isopropanol (tent.)
10B	65	cyclopentane
11	66	2-methylpentane
12	68	3-methylpentane
12A	70	n-butanal
13	71	hexafluorobenzene (eS)
13A	72	n-hexane
13B	72	C_6H_{12} isomer
13C	73	chloroform
14	73	methyl ethyl ketone
15	75	ethyl acetate
16	77	perfluorotoluene (eS)
16A	78	C_6H_{12} isomer
17	79	1,1,1-trichloroethane
18	82	benzene
18A	83	carbon tetrachloride
19	84	cyclohexane
20	85	2-methylhexane
20A	86	2,3-dimethylpentane
20B	87	C_7H_{14} isomer
21	87	3-methylhexane
21A	88	C_7H_{14} isomer
21B	89	C_7H_{14} isomer
22	90	trichloroethylene
23	92	n-heptane
24	95	C_8H_{18} isomer
25	97	methylcyclohexane
26	99	C_8H_{18} isomer
27	102	C_8H_{16} isomer
27A	103	C_8H_{16} isomer
27B	104	$C_6H_{12}O$ isomer
28	105	toluene
29	106	C_8H_{18} isomer
30	108	C_8H_{18} isomer
31	109	C_8H_{16} isomer
32	112	C_8H_{16} isomer
32A	113	C_8H_{16} isomer
33	114	n-octane
34	115	tetrachloroethylene
35A	121	ethylcyclohexane
35B	121	C_9H_{20} isomer
36	122	chlorobenzene
36A	124	C_9H_{18} isomer
37	125	ethylbenzene
38	127	m- and/or p-xylene
39	129	C_9H_{20} isomer
40	130	C_9H_{20} isomer
40A	131	styrene
41	131	o-xylene
42	134	n-nonane
42A	136	$C_{10}H_{20}$ isomer
43	137	$C_{10}H_{22}$ isomer
44	138	$C_{10}H_{22}$ isomer
44A	138	isopropylbenzene
45	139	$C_{10}H_{22}$ isomer
45A	140	$C_{10}H_{20}$ isomer
46	141	$C_{10}H_{22}$ isomer
46A	143	$C_{10}H_{22}$ isomer
47	144	n-propylbenzene
47A	144	benzaldehyde
48	145	m- and/or p-ethyltoluene
48A	146	$C_{10}H_{22}$ isomer
49	146	1,3,5-trimethylbenzene
49A	147	$C_{11}H_{24}$ isomer
50	148	$C_{10}H_{22}$ isomer
51	149	o-ethyltoluene
51A	149	phenol
52	149	$C_{11}H_{24}$ isomer
53	150	$C_{10}H_{22}$ isomer + benzonitrile (tent.)
54	151	1,2,4-trimethylbenzene
55	153	n-decane
56	155	dichlorobenzene isomer
56A	155	C_4-alkyl benzene isomer
57	157	$C_{11}H_{24}$ isomer + 1,2,3-trimethylbenzene
58	159	$C_{11}H_{24}$ isomer
58A	160	indan
59	160	$C_{11}H_{24}$ isomer
59A	161	$C_{10}H_{20}$ isomer

(continued)

Table A20 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
60	162	$C_{11}H_{24}$ isomer	74A	188	$C_{12}H_{24}$ isomer
60A	162	C_4-alkyl benzene isomer	75	190	$C_{13}H_{28}$ isomer
61	163	C_4-alkyl benzene isomer	76	191	$C_{13}H_{28}$ isomer
62	164	acetophenone	76A	191	C_6-alkyl benzene isomer
63	165	$C_{11}H_{24}$ isomer	76B	192	$C_{13}H_{26}$ isomer
64	165	$C_{11}H_{24}$ + $C_{10}H_{18}$ isomers	77	194	unsat. hydrocarbon
64A	166	C_4-alkyl benzene isomer	77A	194	C_6-alkyl cyclohexane isomer
65	168	C_4-alkyl benzene isomer	78	195	$C_{13}H_{28}$ isomer
65A	169	$C_{11}H_{22}$ isomer	79	197	$C_{13}H_{28}$ isomer
65B	173	C_5-alkyl benzene isomer	80	199	$C_{14}H_{30}$ isomer
66	171	*n*-undecane	81	202	*n*-tridecane
66A	172	$C_{11}H_{22}$ isomer	81A	205	β-methylnaphthalene
66B	173	C_5-alkyl benzene isomer	82	205	$C_{15}H_{32}$ isomer
67	174	$C_{12}H_{26}$ isomer	83	207	α-methylnaphthalene
67A	175	$C_{11}H_{20}$ isomer	83A	208	$C_{14}H_{28}$ isomer
68	176	$C_{12}H_{26}$ isomer	84	210	C_7-alkyl cyclohexane isomer
68A	177	C_5-alkyl benzene isomer	85	212	$C_{14}H_{30}$ isomer
69	178	$C_{11}H_{22}$ + $C_{11}H_{20}$ isomers	85A	212	$C_{15}H_{32}$ isomer
70	180	$C_{12}H_{26}$ isomer	86	213	$C_{14}H_{30}$ isomer
70A	181	C_5-alkyl benzene isomer	87	214	$C_{15}H_{32}$ isomer
71	181	$C_{12}H_{26}$ isomer	87A	215	alkyl butyrate
71A	182	C_5-alkyl benzene isomer	87B	216	$C_{14}H_{28}$ isomer
72	183	$C_{12}H_{26}$ isomer	88	217	*n*-tetradecane
72A	183	C_5-alkyl benzene isomer	88A	224	$C_{15}H_{30}$ isomer
73	184	trichlorobenzene isomer	89	225	$C_{15}H_{32}$ isomer
73A	186	$C_{12}H_{24}$ isomer	90	231	*n*-pentadecane
73B	186	naphthalene			
74	187	*n*-dodecane			

[a] See Table 44 for sampling protocol.

Table A21. VAPOR-PHASE ORGANICS IN AMBIENT AIR FROM BEAUMONT, TX (P4/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
1A	44	xenon (traces)
2	47	propene
2A	48	butene isomer
3	49	butadiene
3A	50	C_4H_{10} isomer
3B	51	C_4H_8 isomer
4	51	C_4H_6 isomer
5	53	C_5H_{10} isomer
6	55	isopentane
7A	56	C_5H_{10} isomer
8	57	*n*-pentane
9	58	acetone + C_5H_{10} isomer
10	60	methylene chloride + C_5H_{10} isomer
11	62	C_5H_8 isomer
11A	63	isopropanol
12	64	*t*-butanol
12A	65	C_5H_8 isomer
12B	66	C_5H_{10} isomer
13	67	2-methylpentane
14	70	3-methylpentane
15	71	C_6H_{12} isomer
15A	71	butanal
16	72	hexafluorobenzene (eS)
16A	73	*n*-hexane
17	74	C_6H_{12} isomer + methyl ethyl ketone
17A	74	chloroform (traces)
17B	75	C_6H_{12} isomer
18	77	ethyl acetate
19	78	perfluorotoluene (eS) + C_6H_{12} isomer
19A	79	alcohol (isomer)
19B	80	1,1,1-trichloroethane
19C	82	C_7H_{12} isomer
19D	83	C_6H_{10} isomer
20	83	benzene
20A	84	carbon tetrachloride (traces)
20B	85	cyclohexane
21	86	2-methylhexane
22	88	3-methylhexane
22A	90	C_7H_{14} isomer
23	91	C_7H_{14} isomer + pentanal (tent.)
23A	92	trichloroethylene (traces)
24	93	*n*-heptane
24A	94	C_7H_{14} isomer
24B	94	C_8H_{18} isomer
25	95	diisobutylene
26	96	C_8H_{16} isomer
27	97	methylcyclohexane
28	98	C_8H_{16} isomer
29	100	C_8H_{14} + C_8H_{16} isomers
30	101	C_8H_{16} isomer
30A	103	hexanal
30B	104	C_8H_{14} isomer
30C	105	C_8H_{16} isomer
31	105	toluene
32	107	C_8H_{18} isomer + alcohol (tent.)
32A	108	C_8H_{16} isomer
33	108	C_8H_{18} isomer
34	110	C_8H_{16} isomer
34A	111	C_8H_{18} isomer
35	112	unsat. hydrocarbon
36	114	*n*-octane
36A	115	C_8H_{16} isomer
37	115	tetrachloroethylene
37A	116	C_8H_{16} isomer
37B	117	C_8H_{16} isomer
39	119	C_9H_{20} isomer
40	121	4-vinyl-1-cyclohexene
40A	122	C_9H_{20} isomer
40B	123	C_9H_{18} isomer
41	125	ethylbenzene
41A	125	C_9H_{18} isomer
42	127	*m*- and/or *p*-xylene
42A	127	C_9H_{20} isomer
43	129	C_9H_{20} isomer
44	130	styrene
44A	132	*o*-xylene
44B	133	C_9H_{18} isomer
45	134	*n*-nonane
46	137	C_9H_{18} isomer
47	138	$C_{10}H_{22}$ isomer
47A	138	isopropylbenzene
48	139	C_9H_{16} isomer
49	141	$C_{10}H_{22}$ isomer
49A	142	$C_{10}H_{20}$ isomer
50	143	benzaldehyde
50A	144	*n*-propylbenzene
51	145	*m*- and/or *p*-ethyltoluene
51A	147	$C_{10}H_{22}$ isomer

(continued)

Table A21 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
52	147	$C_{10}H_{22}$ isomer
53	148	$C_{10}H_{22}$ isomer
54	149	*o*-ethyltoluene
55	150	$C_{11}H_{24}$ isomer
56	151	$C_{10}H_{20}$ isomer
56A	152	$C_{10}H_{20}$ isomer
57	152	1,2,4-trimethylbenzene
58	153	$C_{10}H_{20}$ isomer
59	154	*n*-decane
59A	155	$C_{11}H_{24}$ isomer (tent.)
59B	155	C_4-alkyl benzene isomer
59C	156	dichlorobenzene isomer (trace)
60	156	triisobutylene
60A	157	1,2,3-trimethylbenzene
60B	157	C_4-alkyl benzene isomer
61	157	$C_{11}H_{24}$ isomer
62	158	$C_{11}H_{24}$ isomer
62A	159	$C_{10}H_{20}$ isomer
62B	159	indan (traces)
62C	160	C_4-alkyl cyclohexane isomer
63	160	$C_{12}H_{24}$ isomer
64	161	$C_{11}H_{24}$ isomer
64A	162	C_4-alkyl benzene isomer
65	162	C_4-alkyl benzene isomer
65A	163	$C_{12}H_{22}$ isomer (tent.)
66	163	$C_{11}H_{24}$ isomer
66A	165	C_4-alkyl benzene isomer
67	165	$C_{11}H_{24}$ isomer (tent.)
67A	166	acetophenone
68	167	C_4-alkyl benzene isomer
69	168	C_4-alkyl benzene isomer
69A	169	$C_{11}H_{22}$ isomer
70	171	*n*-undecane
71	172	alcohol or unknown
72	174	sat. hydrocarbon
72A	174	C_4-alkyl benzene isomer
73	175	$C_{13}H_{26}$ isomer
73A	175	$C_{11}H_{20}$ isomer
74	177	unsat. hydrocarbon
75	178	sat. hydrocarbon (tent.)
76A	180	$C_{12}H_{24}$ isomer
77	182	$C_{13}H_{28}$ isomer
78	185	$C_9H_{18}O$ isomer (tent.)
78A	186	naphthalene
79	187	*n*-dodecane
79A	190	sat. hydrocarbon
80	191	$C_{12}H_{24}$ isomer
81	202	*n*-tridecane
81A	205	methylnaphthalene isomer
83	208	tetraisobutylene
84	209	$C_{13}H_{26}$ isomer
84A	211	$C_{14}H_{30}$ isomer
85	214	alkyl butyrate
86	216	$C_{14}H_{30}$ isomer

[a] See Table 44 for sampling protocol.

Table A22. VAPOR-PHASE ORGANICS IDENTIFIED IN AMBIENT AIR FROM BEAUMONT, TX VICINITY (P3/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2
3	47	propane
3A		C_4H_8 isomer
3B	49	C_4H_6 isomer
4	49	C_4H_{10} isomer
4A	50	acetaldehyde (tent.)
4B	51	C_4H_8 isomer
4C	55	isopentane
6	57	*n*-pentane + acetone
7	60	methylene chloride
8A	63	isopropanol (tent.)
8B	67	cyclopentane
9	67	2-methylpentane
10	69	3-methylpentane
11	71	hexafluorobenzene (eZ)
12	72	*n*-hexane
13	73	methyl ethyl ketone + chloroform
14	76	ethyl acetate
15	77	perfluorotoluene (eZ)
15A	78	methylcyclopentane
16	80	1,1,1-trichloroethane
17	83	benzene
17A	84	carbon tetrachloride (traces)
18	85	cyclohexane
19	86	2-methylhexane
19A	87	2,3-dimethylpentane
20	88	3-methylhexane
20A	89	alcohol (tent.)
21	89	1,2-dichloropropane
22	90	C_7H_{14} isomer
22A	91	trichloroethylene
23	93	*n*-heptane
24	95	C_8H_{16} isomer
25	98	methylcyclohexane
25A	99	C_8H_{16} isomer
26	100	C_8H_{18} isomer
26A	101	C_8H_{16} isomer
26B	102	C_8H_{18} isomer
27	102	C_8H_{16} isomer
28	103	C_8H_{18} isomer
28A	104	$C_6H_{12}O$ isomer
29	105	toluene
30	107	C_8H_{18} isomer
31	109	C_8H_{18} isomer
32	110	C_8H_{16} isomer
32A	112	C_8H_{16} isomer
33	114	*n*-octane
33A	114	C_8H_{16} isomer
34	115	tetrachloroethylene
34A	120	C_9H_{20} isomer
35A	121	C_9H_{18} isomer
35B	121	C_8H_{16} isomer
35C	121	C_9H_{20} isomer
36	122	chlorobenzene
36A	124	C_9H_{18} isomer
37	125	ethylbenzene
37A	126	C_9H_{18} isomer
38	127	*m*- and/or *p*-xylene
38A	129	phenylacetylene (traces)
38B	129	C_9H_{20} isomer
39	130	$C_{10}H_{22}$ isomer
39A	131	C_9H_{18} isomer
39B	131	styrene
40	132	*o*-xylene
40A	133	C_9H_{18} isomer
41	134	*n*-nonane
41A	136	C_9H_{18} isomer
41B	137	$C_{10}H_{20}$ isomer
42	138	$C_{10}H_{22}$ isomer
42A	139	isopropylbenzene
42B	140	$C_{10}H_{20}$ isomer
43	141	$C_{10}H_{22}$ isomer
43A	142	$C_{10}H_{20}$ isomer
43B	143	sat. hydrocarbon
43C	144	$C_{10}H_{20}$ isomer
43D	145	*n*-propylbenzene
44	145	$C_{10}H_{22}$ + ethyltoluene isomers
44A	146	benzaldehyde
45	147	$C_{11}H_{24}$ isomer
45A	148	$C_{10}H_{22}$ isomer
45B	148	$C_{11}H_{24}$ isomer
46	149	phenol + benzonitrile
47	150	$C_{10}H_{22}$ isomer
48	151	C_3-alkyl benzene isomer + benzofuran
49	153	*n*-decane
49A	156	dichlorobenzene isomer
50	154	$C_{10}H_{20}$ isomer
50A	156	$C_{11}H_{24}$ isomer
51	157	1,2,3-trimethylbenzene + $C_{11}H_{24}$ isomer

(continued)

Table A22 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
52	158	$C_{11}H_{24}$ isomer
52A	159	dichlorobenzene isomer
53	160	$C_{11}H_{24}$ isomer
53A	160	$C_{10}H_{20}$ isomer
54	161	$C_{11}H_{24}$ isomer
54A	162	C_4-alkyl benzene isomer
54B	162	C_4-alkyl benzene isomer
55	163	acetophenone
56	165	$C_{11}H_{24}$ isomer
56A	168	$C_{11}H_{24}$ isomer
56B	169	$C_{11}H_{22}$ isomer
57	171	*n*-undecane
58	175	$C_{12}H_{26}$ isomer
58A	179	$C_{11}H_{22}$ isomer
59A	185	$C_{12}H_{24}$ isomer
60	187	naphthalene
60A	189	*n*-dodecane
60B	196	$C_{13}H_{28}$ isomer
60C	202	$C_{13}H_{26}$ isomer
60D	204	*n*-tridecane
60E	207	methylnaphthalene isomer
61	214	alkyl butyrate
61A	217	biphenyl
61B	219	diphenyl ether
61C	220	$C_{14}H_{30}$ isomer
61D	230	$C_{15}H_{30}$ isomer
61E	231	$C_{15}H_{32}$ isomer

[a] See Table 44 for sampling protocol.

Table A23. VAPOR-PHASE ORGANICS IDENTIFIED IN AMBIENT AIR FROM BEAUMONT, TX VICINITY (P5/L1)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2
1A	43	xenon
2A	47	C_4H_8 isomer
2B	48	C_4H_{10} isomer
3	49	acetaldehyde
3A	54	isopentane
4	56	acetone
6	59	methylene chloride
6A	61	isopropanol
6B	65	cyclopentane
7	66	2-methylpentane
8	68	3-methylpentane
9	70	hexafluorobenzene (eS)
9A	71	*n*-hexane
9B	72	chloroform
9C	72	C_6H_{12} isomer
9D	74	ethyl acetate
9E	76	C_7H_{16} isomer
10	76	perfluorotoluene (eS)
10A	77	methylcyclopentane
10B	78	1,2-dichloroethane
11	79	C_7H_{16} isomer
11A	79	1,1,1-trichloroethane
11B	82	C_6H_{10} isomer
12	83	benzene
12A	84	carbon tetrachloride
12B	84	cyclohexane
13	85	2-methylhexane
13A	86	2,3-dimethylpentane
14	87	3-methylhexane
14A	88	alcohol (tent.)
15	90	C_7H_{14} isomer
15A	91	trichloroethylene
16	92	*n*-heptane
16A	93	C_7H_{14} isomer
17	95	C_8H_{16} isomer
18	98	methylcyclohexane
18A	99	C_8H_{16} isomer
18B	100	C_8H_{16} isomer
19	100	C_8H_{18} isomer
20	102	C_8H_{18} isomer
20A	103	alkyl acid
21	104	C_8H_{18} isomer
22	105	toluene
23	107	C_8H_{18} isomer
24	109	C_8H_{18} isomer
25	110	C_8H_{16} isomer
25A	112	C_8H_{16} isomer
25B	113	1,2-dibromoethane
26	114	*n*-octane
27	115	tetrachloroethylene
27A	119	C_9H_{20} isomer
27B	121	C_9H_{20} isomer
27C	122	C_9H_{18} isomer
29	122	C_8H_{16} isomer
29A	123	C_9H_{18} isomer
29B	125	C_9H_{18} isomer
30	126	ethylbenzene
30A	127	C_9H_{18} isomer
30B	127	C_9H_{20} isomer
31	128	*m*- and/or *p*-xylene
31A	128	C_9H_{20} isomer
32	129	C_9H_{20} isomer
32A	130	C_9H_{20} isomer
33	131	$C_{10}H_{22}$ isomer
33A	132	styrene (traces)
34	132	$C_{10}H_{22}$ isomer
34A	133	*o*-xylene
34B	134	C_9H_{18} isomer
35	135	*n*-nonane
35A	135	$C_{10}H_{22}$ isomer
35B	136	$C_{10}H_{20}$ isomer
35C	137	$C_{10}H_{22}$ isomer
36	138	$C_{10}H_{22}$ isomer
36A	139	isopropylbenzene (traces)
37	140	$C_{10}H_{22}$ isomer
37A	141	$C_{10}H_{20}$ isomer
38	141	$C_{11}H_{24}$ isomer
38A	142	$C_{10}H_{20}$ isomer
38B	142	$C_{10}H_{16}$ isomer
38C	143	$C_{10}H_{20}$ isomer
38D	144	*n*-propylbenzene
38E	145	$C_{10}H_{22}$ isomer
39	145	ethyltoluene isomer
40	147	$C_{11}H_{24}$ isomer
40A	148	benzaldehyde
41	149	C_4-alkyl benzene isomer
42	150	$C_{11}H_{24}$ isomer
43	151	$C_{11}H_{24}$ isomer
44	152	1,2,4-trimethylbenzene
44A	153	$C_{10}H_{20}$ isomer
45	154	*n*-decane

(continued)

Table A23 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
46	155	$C_{11}H_{24}$ isomer
46A	155	$C_{11}H_{22}$ isomer
46B	156	dichlorobenzene isomer
47	156	$C_{11}H_{24}$ isomer
48	157	1,2,3-trimethylbenzene + $C_{11}H_{24}$ isomer
49	159	$C_{12}H_{26}$ isomer
49A	160	$C_{10}H_{20}$ isomer
50	160	$C_{12}H_{26}$ isomer
50A	161	$C_{11}H_{22}$ isomer
51	161	$C_{12}H_{26}$ isomer
51A	162	C_4-alkyl benzene isomer
51B	162	$C_{11}H_{22}$ isomer
52	163	C_4-alkyl benzene isomer
52A	164	C_4-alkyl benzene isomer
53	165	sat. hydrocarbon
54	166	sat. hydrocarbon
54A	167	C_4-alkyl benzene isomer
54B	168	acetophenone
55	169	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
55A	170	$C_{11}H_{22}$ isomer
55B	171	C_4-alkyl benzene isomer
56	171	*n*-undecane
56A	173	C_4-alkyl benzene isomer
56B	174	$C_{12}H_{24}$ isomer
57	175	$C_{12}H_{26}$ isomer
57A	175	C_4-alkyl benzene isomer
58	177	C_5-alkyl benzene + unsat. hydrocarbon
59A	180	C_5-alkyl benzene isomer
59B	181	$C_{12}H_{26}$ isomer
59C	182	$C_{12}H_{24}$ isomer
59D	187	naphthalene
60	188	*n*-dodecane
61	192	unsat. hydrocarbon
62	202	$C_{14}H_{30}$ isomer
63	214	alkyl butyrate

[a] See Table 44 for sampling protocol.

Table A24. VAPOR-PHASE ORGANICS IDENTIFIED IN AMBIENT AIR FROM BEAUMONT, TX VICINITY (P6/L2)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
1A	44	xenon (traces)
3	47	propane
3A	49	C_4H_8 isomer
4	49	isobutane
4A	51	C_4H_8 isomer
4B	52	*n*-butane
4C	52	acetaldehyde
4D	54	isopentane
6	56	acetone
8	59	methylene chloride
8B	63	isopropanol (tent)
9	66	2-methylpentane
10	69	3-methylpentane
10A	70	C_6H_{12} isomer (tent)
11	71	hexafluorobenzene (eS)
12	72	*n*-hexane
13	73	chloroform
13A	74	methyl ethyl ketone
13B	76	ethyl acetate
14	77	perfluorotoluene (eS) + methylcyclopentane
14A	80	1,1,1-trichloroethane
15	82	benzene
15A	83	carbon tetrachloride
15B	84	cyclohexane
16	85	2-methylhexane
16A	86	2,3-dimethylpentane
17	87	3-methylhexane
17A	89	C_7H_{14} isomer
17B	90	trichloroethylene
17C	91	C_7H_{14} isomer
18	92	*n*-heptane
19	97	methylcyclohexane
19A	98	C_8H_{16} isomer
19B	99	C_8H_{18} isomer
19C	100	C_8H_{18} isomer
19D	101	C_8H_{16} isomer
20	104	toluene
21	106	C_8H_{18} isomer
22	108	C_8H_{18} isomer
22A	109	C_8H_{16} isomer
22B	111	C_8H_{16} isomer
23	113	*n*-octane
24	115	tetrachloroethylene
25	117	hexamethylcyclotrisiloxane
25A	119	C_9H_{20} isomer
26	121	ethylcyclohexane
27	126	ethylbenzene
27A	126	C_9H_{20} isomer
28	127	*m*- and/or *p*-xylene
28A	129	C_9H_{20} isomer
29	130	$C_{10}H_{22}$ isomer
30	132	$C_{10}H_{22}$ isomer
30A	132	*o*-xylene
30B	133	C_9H_{18} isomer
31	134	*n*-nonane
31A	136	$C_{10}H_{20}$ isomer
32	137	$C_{10}H_{22}$ isomer
33	138	$C_{10}H_{22}$ isomer
33A	138	unsaturated hydrocarbon
34	139	$C_{10}H_{22}$ isomer
34A	140	$C_{10}H_{20}$ isomer
35	141	$C_{10}H_{22}$ isomer
35A	141	$C_{10}H_{20}$ isomer
35B	143	$C_{10}H_{20}$ isomer
35C	144	*n*-propylbenzene
35D	145	$C_{10}H_{20}$ isomer
36	145	$C_{10}H_{22}$ isomer
36A	146	ethyltoluene isomer
36B	146	benzaldehyde
37	147	$C_{11}H_{24}$ isomer
38	149	$C_{11}H_{24}$ isomer
39	150	$C_{11}H_{24}$ isomer
40	152	octamethylcyclotetrasiloxane
40A	152	C_3-alkylbenzene isomer
41	153	*n*-decane
41A	154	phenol
42	154	$C_{11}H_{24}$ isomer
42A	155	$C_{11}H_{22}$ isomer
42B	155	dichlorobenzene isomer (trace)
43	157	$C_{11}H_{24}$ isomer
44	158	$C_{12}H_{26}$ isomer
45	160	$C_{11}H_{24}$ or saturated hydrocarbon
45A	160	unsaturated hydrocarbon
46	161	saturated hydrocarbon
46A	163	$C_{11}H_{22}$ isomer
47	165	saturated hydrocarbon
47A	166	acetophenone
47B	168	$C_{11}H_{22}$ isomer
48	171	*n*-undecane
48A	179	$C_{12}H_{24}$ isomer

(continued)

Table A24 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
49	180	silane compound
49A	180	$C_{12}H_{26}$ isomer
49B	182	$C_{12}H_{24}$ isomer
49C	184	trichlorobenzene isomer
49D	186	naphthalene
50	187	*n*-dodecane
50A	189	$C_{13}H_{26}$ isomer
51	191	$C_{13}H_{26}$ isomer
52	194	silane compound
53	202	*n*-tridecane
54	207	silane compound
55	214	alkyl butyrate
56	217	*n*-tetradecane
56A	224	$C_{15}H_{30}$ isomer
57	226	*n*-pentadecane
58	228	silane compound
58A	229	$C_{15}H_{30}$ isomer

[a] See Table 44 for sampling protocol.

Part IV - HOUSTON, TX

Table A25. VAPOR-PHASE ORGANICS IDENTIFIED IN AMBIENT AIR FROM HOUSTON, TX (P9/L2)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	52	CO_2
3A	55	acetaldehyde
3B	56	C_4H_8 isomer
4	56	C_4H_{10} isomer
5	58	n-butane
6	60	isopentane
7	61	acetone
8	62	n-pentane
8A	62	C_5H_8 isomer
9	64	methylene chloride
9A	66	cyclopentadiene or C_5H_6 isomer
10	68	butenal isomer
10A	69	cyclopentane
11	70	2-methylpentane
11A	71	methyl vinyl ketone
11B	71	n-butanal
12	72	methyl ethyl ketone
12A	72	3-methylpentane
12B	73	C_6H_{12} isomer
13	74	hexafluorobenzene (cS)
14	75	n-hexane
14A	75	alcohol (tent.)
14B	76	chloroform (traces)
15	78	isobutanol
16	80	perfluorotoluene (eS)
16A	80	methylcyclopentane
16B	81	1,2-dichloroethane
17	82	1,1,1-trichloroethane
17A	84	$C_5H_{10}O$ isomer (tent.)
17B	85	dichloropropene isomer (tent.)
18	86	benzene
18A	87	C_7H_{14} isomer
19	87	carbon tetrachloride
19A	88	cyclohexane
20	91	2-methylhexane
20A	91	2,3-dimethylpentane
21	93	3-methylhexane
21A	93	1,2-dichloropropane (traces)
22	94	ethyl acrylate
23	96	trichloroethylene
23A	97	C_8H_{18} isomer (tent.)
24	98	methyl methacrylate
24A	98	n-heptane
25	101	C_8H_{16} isomer (tent.)
26	104	4-methyl-2-pentanone
26A	106	C_8H_{16} isomer
27	107	C_8H_{18} isomer
28	111	4-methyl-2-pentanol
29	113	toluene
29A	115	C_8H_{16} isomer
30	116	C_8H_{18} isomer
30A	117	$C_6H_{12}O$ isomer (tent.)
31	118	C_8H_{18} isomer
32	119	C_8H_{16} isomer
32A	120	hexanal (traces)
33	121	C_8H_{16} isomer
34	124	n-octane
35	125	tetrachloroethylene
35A	126	C_8H_{16} isomer
35B	129	C_9H_{18} isomer
36	131	C_9H_{20} isomer
37	133	C_9H_{20} isomer
37A	133	chlorobenzene
37B	134	ethylcyclohexane
37C	134	C_9H_{18} isomer
38	135	C_9H_{20} isomer
38A	136	C_9H_{18} isomer
38B	137	C_9H_{18} isomer
39	138	ethylbenzene
39A	139	C_9H_{18} isomer
40	141	m- and/or p-xylene
40A	141	$C_{10}H_{20}$ isomer
41	142	C_9H_{20} isomer
41A	143	C_9H_{18} isomer
41B	143	$C_9H_{14}O$ isomer
42	144	C_9H_{20} isomer
42A	145	$C_{10}H_{20}$ isomer
43	145	styrene + butyl acrylate
43A	156	C_9H_{18} isomer
44	147	o-xylene
45	148	C_9H_{18} isomer
45A	149	1,3-dichloropropene
45B	149	C_9H_{18} isomer
45C	150	$C_{10}H_{22}$ isomer
45D	150	$C_{10}H_{20}$ isomer
46	151	n-nonane
46A	153	$C_{10}H_{20}$ isomer
46B	154	$C_{10}H_{20}$ isomer
47	155	isopropylbenzene
47A	156	$C_{10}H_{22}$ isomer
48	157	isobutyl methacrylate
48A	158	$C_{10}H_{22}$ isomer

(continued)

Table A25 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
48B	159	$C_{10}H_{20}$ isomer
48C	160	propylcyclohexane
48D	160	$C_{10}H_{20}$ isomer
49	161	benzaldehyde + $C_{10}H_{22}$ isomer
49A	162	$C_{11}H_{24}$ isomer
49B	162	$C_{10}H_{20}$ isomer
50	163	*n*-propylbenzene
50A	164	$C_{10}H_{20}$ isomer
51	165	*m*- and/or *p*-ethyltoluene
51A	166	$C_{10}H_{22}$ isomer
51B	167	1,3,5-trimethylbenzene
52	168	*n*-butyl methacrylate
52A	169	$C_{11}H_{24}$ isomer
52B	170	*o*-ethyltoluene
53	170	C_9H_{18} isomer
53A	171	phenol
53B	171	$C_{10}H_{22}$ isomer
54	172	$C_{11}H_{24}$ isomer
54A	173	*n*-octanal + C_3H_5-benzene isomer
55	173	1,2,4-trimethylbenzene
55A	174	$C_{10}H_{20}$ isomer
55B	175	$C_{11}H_{22}$ isomer
56	175	unsaturated hydrocarbon
56A	176	dichlorobenzene isomer (trace)
57	176	*n*-decane
58	177	$C_{11}H_{22}$ isomer
58A	179	$C_{11}H_{22}$ isomer
58B	180	1,2,3-trimethylbenzene
58C	180	$C_{11}H_{24}$ isomer
59	180	$C_{11}H_{22}$ + C_4-alkyl benzene isomers
60	181	$C_{11}H_{24}$ isomer
60A	182	$C_{11}H_{22}$ isomer
60B	183	$C_{11}H_{22}$ isomer
61	183	$C_{11}H_{24}$ isomer
61A	185	$C_{11}H_{22}$ isomer
62	185	C_4-alkyl cyclohexane isomer
62A	185	$C_{11}H_{24}$ isomer
63	187	acetophenone + $C_{11}H_{24}$ isomer
63A	187	$C_{11}H_{20}$ isomer
63B	188	C_4-alkyl benzene isomer
63C	189	$C_{12}H_{24}$ isomer
63D	189	$C_{12}H_{26}$ isomer
63E	191	C_4-alkyl benzene isomer
63F	191	$C_{10}H_{18}$ isomer
64	191	$C_{11}H_{24}$ isomer
64A	192	$C_{12}H_{26}$ isomer
64B	193	C_4-alkyl benzene isomer
65	194	$C_{12}H_{24}$ isomer
65A	195	$C_{11}H_{22}$ isomer
65B	195	C_4-alkyl benzene isomer
66	197	*n*-nonanal
67	199	saturated hydrocarbon (tent.)
67A	200	$C_{12}H_{24}$ isomer
68	200	*n*-undecane
68A	202	$C_{12}H_{24}$ isomer
69	203	$C_{12}H_{24}$ + C_4-alkyl benzene isomers
69A	204	C_4-alkyl benzene isomer
69B	205	$C_{12}H_{24}$ isomer
70	205	$C_{12}H_{26}$ isomer
70A	209	C_5-alkyl benzene isomer
70B	209	C_5-alkyl cyclohexane isomer
70C	210	$C_{12}H_{24}$ isomer
70D	213	$C_{12}H_{26}$ isomer
70E	214	C_5-alkyl benzene isomer
70F	215	$C_{12}H_{26}$ isomer
70G	216	C_5-alkyl benzene isomer
70H	216	saturated hydrocarbon
71	217	naphthalene
71A	219	$C_{12}H_{24}$ isomer
72	220	*n*-decanal
72A	221	C_6-alkyl benzene isomer
73	222	*n*-dodecane
73A	224	unsaturated hydrocarbon
73B	227	$C_{13}H_{26}$ isomer
73C	238	saturated hydrocarbon
73D	239	alcohol (tent.)
73E	240	$C_{13}H_{26}$ isomer
74	240	*n*-tridecane
74A	240	methylnaphthalene isomer

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[a] See Table 45 for sampling protocol.

Table A26. VAPOR-PHASE ORGANICS IDENTIFIED IN AMBIENT AIR FROM HOUSTON, TX (P11/L3)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	50	CO_2
2A	54	propane (tent.)
2B	55	C_4H_8 isomer
2C	57	C_4H_8 isomer
3	58	C_4H_{10} isomer
3A	58	isopentane
4	59	acetone
5	61	n-pentane
5A	62	C_5H_{10} isomer
6	63	methylene chloride
6A	66	C_4H_8O isomer (tent.)
6B	68	C_6H_{14} isomer (tent.)
6C	69	cyclopentane
7	69	2-methylpentane
7A	70	butanal
7B	70	methyl vinyl ketone (tent.)
8	71	methyl ethyl ketone + 3-methylpentane
8A	72	C_6H_{12} isomer
9	73	hexafluorobenzene (eI)
9A	74	n-hexane
10	75	chloroform
10A	78	C_6H_{12} isomer
11	80	perfluorotoluene (eI)
11A	80	methylcyclopentane
11B	82	1,1,1-trichloroethane
12	85	benzene
12A	86	C_7H_{14} isomer
12B	86	carbon tetrachloride
12C	87	cyclohexane
13	90	2-methylhexane
14	93	3-methylhexane
14A	94	pentanal
14B	95	C_7H_{14} isomer
15	96	trichloroethylene
16	99	n-heptane
16A	101	C_7H_{14} isomer
16B	102	C_8H_{18} isomer
17	105	methylcyclohexane
17A	106	$C_6H_{12}O$ isomer
17B	106	C_8H_{16} isomer
18	108	C_8H_{18} isomer
18A	110	C_8H_{16} isomer
18B	112	C_8H_{16} isomer
19	114	toluene
19A	116	C_8H_{16} isomer
20	117	C_8H_{18} isomer
20A	118	$C_6H_{12}O$ isomer
21	119	C_8H_{18} isomer
22	120	C_8H_{16} isomer
22A	121	C_8H_{18} isomer
22B	123	C_8H_{16} isomer
22C	125	n-octane
23	126	tetrachloroethylene
23A	132	C_9H_{20} isomer
23B	133	C_9H_{20} isomer
23C	134	chlorobenzene (traces)
23D	135	ethylcyclohexane
23E	135	C_9H_{20} isomer
23F	136	C_9H_{18} isomer
24	140	ethylbenzene
24A	141	C_9H_{18} isomer
25	142	m- and/or p-xylene
25A	143	C_9H_{20} isomer
26	144	C_9H_{20} isomer
26A	145	$C_7H_{14}O$ isomer
27	145	C_9H_{20} isomer
27A	147	styrene
27B	147	C_9H_{18} isomer
27C	148	C_9H_{20} isomer
28	148	o-xylene
28A	149	C_9H_{18} isomer
28B	150	$C_{10}H_{22}$ isomer
29	150	C_9H_{18} isomer
30	153	n-nonane
30A	155	$C_{10}H_{20}$ isomer
30B	155	C_9H_{18} isomer
30C	157	isopropylbenzene
30D	157	$C_{10}H_{20}$ isomer
31	158	$C_{10}H_{22}$ isomer
31A	158	$C_{10}H_{16}$ isomer (tent.)
31B	160	$C_{10}H_{22}$ isomer
31C	161	propylcyclohexane
31D	162	$C_{10}H_{22}$ isomer
32	163	$C_{10}H_{16}$ isomer + benzaldehyde
32A	163	$C_{10}H_{22}$ isomer
32B	164	$C_{10}H_{20}$ isomer
33	165	$C_{10}H_{22}$ isomer + n-propylbenzene
33A	165	$C_{10}H_{22}$ isomer
34	167	m- and/or p-ethyltoluene
34A	168	benzonitrile (traces)

(continued)

Table A26 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
34B	169	1,3,5-trimethylbenzene	44	203	*n*-undecane
34C	169	$C_{10}H_{22}$ isomer	44A	204	$C_{12}H_{26}$ isomer
34D	170	$C_{10}H_{20}$ isomer	44B	205	C_5-alkyl benzene isomer
35	170	$C_{11}H_{24}$ isomer	44C	206	C_4-alkyl benzene isomer
35A	171	*o*-ethyltoluene + phenol	44D	207	$C_{12}H_{26}$ isomer
36	172	$C_{10}H_{22}$ isomer	44E	209	unsat. hydrocarbon
36A	173	$C_{10}H_{16}$ isomer	44F	209	$C_{12}H_{26}$ isomer
37	173	$C_{11}H_{24}$ isomer	44G	213	unsat. hydrocarbon
38	175	1,2,4-trimethylbenzene	44H	216	C_5-alkyl benzene isomer
38A	176	$C_{10}H_{20}$ isomer	44I	217	$C_{12}H_{26}$ isomer
38B	177	$C_{11}H_{22}$ isomer	44J	220	naphthalene
38C	178	dichlorobenzene isomer (trace)	44K	221	$C_{12}H_{24}$ isomer
39	179	*n*-decane	44L	222	$C_{12}H_{24}$ isomer
39A	181	$C_{11}H_{24}$ isomer	45	224	*n*-dodecane
39B	182	1,2,3-trimethylbenzene	45A	228	unsat. hydrocarbon
39C	183	C_4-alkyl benzene isomer	45B	231	sat. hydrocarbon
40	183	$C_{11}H_{24}$ isomer	45C	236	$C_{13}H_{26}$ isomer
40A	184	$C_{11}H_{24}$ isomer	45D	238	$C_{13}H_{28}$ isomer
41	185	$C_{11}H_{24}$ isomer	45E	240	$C_{13}H_{28}$ isomer
41A	186	C_4-alkyl cyclohexane isomer	46	240	*n*-tridecane
41B	188	sat. hydrocarbon	46A	240	methylnaphthalene isomer (traces)
42	189	acetophenone	46B	240	$C_{14}H_{30}$ isomer
42A	191	C_4-alkyl benzene isomer	46C	240	$C_{15}H_{32}$ isomer
42B	191	$C_{11}H_{22}$ isomer	46D	240	$C_{14}H_{28}$ isomer
42C	192	$C_{11}H_{22}$ isomer	46E	240	*n*-tetradecane
43	193	$C_{11}H_{24}$ isomer	46F	240	$C_{15}H_{32}$ isomer
43A	195	C_4-alkyl benzene isomer	47	240	*n*-pentadecane
43B	197	C_4-alkyl benzene isomer	47A	240	$C_{15}H_{30}$ isomer
43C	199	$C_{11}H_{22}$ isomer			
43D	201	$C_{11}H_{22}$ isomer			

[a] See Table 45 for sampling protocol.

Table A27. VAPOR-PHASE ORGANICS IDENTIFIED IN AMBIENT AIR FROM HOUSTON, TX (P13/L4)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2A	45	xenon (traces)
3	47	acetaldehyde
3A	47	C_4H_8 isomer
4	49	C_4H_8 + C_4H_{10} isomers (tent.)
5	51	isopentane
5A	51	acetone
5B	52	furan (tent.)
5C	52	C_5H_{10} isomer
6	52	*n*-pentane
6A	53	C_5H_{10} isomer
7	54	methylene chloride
8	56	C_6H_{14} isomer
9	56	C_5H_{10} isomer (tent.)
10	58	crotonaldehyde
10A	59	cyclopentane
11	59	2-methylpentane
11A	60	butanal
12	61	3-methylpentane
12A	62	C_6H_{12} isomer
13	62	perfluorobenzene (eH)
14	63	*n*-hexane
14A	64	C_6H_{10} isomer
14B	64	C_6H_{12} isomer
14C	65	C_7H_{16} isomer
14D	66	C_6H_{12} isomer
15	67	perfluorotoluene (eH) + methylcyclopentane
16	69	1,1,1-trichloroethane
17	70	C_7H_{14} isomer
18	72	benzene
18A	73	carbon tetrachloride (traces)
19	74	cyclohexane
20	75	2-methylhexane
20A	76	2,3-dimethylpentane
20B	76	C_7H_{14} isomer
21	77	3-methylhexane
21A	78	C_7H_{14} isomer
22	78	C_7H_{14} isomer
23	79	C_7H_{14} isomer
23A	79	C_8H_{18} isomer
24	81	*n*-heptane
24A	82	C_7H_{14} isomer
25	85	methylcyclohexane
25A	86	C_8H_{16} isomer
25B	86	C_8H_{18} isomer
25C	87	C_8H_{16} isomer
26	87	C_8H_{18} isomer
27	89	C_8H_{16} isomer
27A	91	C_8H_{18} isomer
28	92	toluene
29	94	C_8H_{18} isomer
29A	94	$C_6H_{12}O$ isomer (tent.)
30	95	C_8H_{18} isomer
31	96	C_8H_{16} isomer
32	97	C_9H_{20} isomer
33	98	C_8H_{16} isomer
33A	99	C_8H_{14} isomer
33B	99	C_8H_{16} isomer
34	101	*n*-octane
34A	101	tetrachloroethylene
34B	102	C_8H_{16} isomer
35	103	C_8H_{16} isomer
35A	105	C_9H_{20} isomer
36	105	C_9H_{20} isomer
37	107	C_9H_{20} isomer
37A	107	chlorobenzene
38	107	ethylcyclohexane
39	108	C_8H_{18} isomer
39A	108	$C_7H_{14}O$ isomer (tent.)
39B	109	C_9H_{18} isomer
40	110	C_9H_{18} isomer
41	111	ethylbenzene
41A	112	C_9H_{18} isomer
42	113	*m*- and/or *p*-xylene
43	114	C_9H_{20} isomer
44	115	C_9H_{20} isomer
44A	116	C_9H_{18} isomer
45	116	styrene
45A	117	$C_{10}H_{22}$ isomer
46	117	*o*-xylene
47	119	C_9H_{18} isomer
47A	120	C_9H_{18} isomer
47B	120	C_9H_{16} isomer
48	121	*n*-nonane
49	123	C_9H_{18} isomer
50	124	isopropylbenzene + $C_{10}H_{22}$ isomer
51	125	$C_{10}H_{22}$ isomer
51A	126	$C_{10}H_{20}$ isomer
52	126	$C_{10}H_{22}$ isomer
53	127	propylcyclohexane

(continued)

Table A27 (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
53A	128	$C_{10}H_{22}$ isomer
54	128	benzaldehyde
54A	129	$C_{10}H_{20}$ isomer
54B	129	$C_{10}H_{22}$ isomer
54C	129	$C_{10}H_{20}$ isomer
55	130	*n*-propylbenzene
55A	131	$C_{10}H_{20}$ isomer
56	131	*m*- and/or *p*-ethyltoluene
56A	132	$C_{10}H_{22}$ isomer
57	132	1,3,5-trimethylbenzene
57A	133	$C_{10}H_{20}$ isomer
57B	133	$C_{10}H_{20}$ isomer
58	133	$C_{11}H_{24}$ isomer
58A	134	phenol
59	134	*o*-ethyltoluene
59A	134	$C_{10}H_{22}$ isomer
59B	135	$C_{10}H_{20}$ isomer
60	135	$C_{11}H_{24}$ isomer
60A	136	C_3H_5-benzene isomer
61	137	1,2,4-trimethylbenzene
61A	137	$C_{10}H_{20}$ isomer
61B	138	$C_{10}H_{20}$ isomer
62	140	*n*-decane
62A	140	C_4-alkyl benzene isomer
62B	141	$C_{11}H_{22}$ isomer
62C	142	C_4-alkyl benzene isomer
63	142	1,2,3-trimethylbenzene
63A	143	$C_{11}H_{24}$ isomer
63B	143	$C_{11}H_{24}$ isomer
64	144	$C_{11}H_{24}$ isomer + indan
65	145	$C_{11}H_{24}$ isomer
65A	146	C_4-alkyl cyclohexane isomer
66	146	$C_{11}H_{24}$ isomer
66A	147	$C_{11}H_{22}$ isomer
66B	147	C_4-alkyl benzene isomer
66C	147	$C_{11}H_{24}$ isomer
67	148	acetophenone
67A	148	C_4-alkyl benzene isomer
68	149	C_4-alkyl benzene isomer
68A	142	$C_{11}H_{22}$ isomer
68B	150	$C_{11}H_{24}$ isomer
68C	150	$C_{11}H_{22}$ isomer
68D	150	$C_{11}H_{24}$ isomer
68E	151	C_4-alkyl benzene isomer
69	151	$C_{11}H_{24}$ isomer
69A	152	$C_{11}H_{24}$ isomer
70	153	C_4-alkyl benzene isomer
70A	153	C_4H_7-benzene isomer
70B	153	$C_{11}H_{22}$ isomer
71	154	C_4-alkyl benzene isomer
71A	154	C_4H_7-benzene isomer
71B	154	$C_{11}H_{22}$ isomer
72	155	*n*-nonanal
72A	155	$C_{11}H_{24}$ isomer
72B	157	$C_{11}H_{22}$ isomer
72C	157	C_5-alkyl benzene isomer
73	157	*n*-undecane
73A	158	$C_{12}H_{24}$ isomer
73B	159	tetramethylbenzene isomer
74	160	C_4-alkyl benzene isomer
74A	160	$C_{12}H_{24}$ isomer
75	163	C_5-alkyl benzene isomer
75A	163	$C_{12}H_{24}$ isomer
75B	164	C_5-alkyl benzene isomer
76	165	C_5-alkyl benzene + $C_{12}H_{24}$ isomers
76A	167	C_5-alkyl benzene isomer
77	167	$C_{12}H_{26}$ isomer
77A	168	$C_{12}H_{26}$ isomer
77B	169	C_5-alkyl benzene isomer
78	170	naphthalene
78A	171	$C_{12}H_{24}$ isomer
78B	172	C_6-alkyl benzene isomer (traces)
79	173	*n*-decanal
79A	173	$C_{12}H_{24}$ isomer
79B	173	$C_{12}H_{22}$ isomer
79C	173	$C_{12}H_{24}$ isomer
80	174	*n*-dodecane
81	177	$C_{13}H_{28}$ isomer
81A	177	C_6-alkyl benzene isomer
81B	178	$C_{13}H_{26}$ isomer
81C	178	$C_{13}H_{28}$ isomer
81D	180	$C_{12}H_{24}$ isomer
81E	181	C_6-alkyl benzene isomer
81F	182	$C_{13}H_{26}$ isomer
82	184	$C_{13}H_{28}$ isomer
82A	186	$C_{13}H_{26}$ isomer
83	187	N,N-di-*n*-butyl formamide (tent.)
83A	189	methylnaphthalene isomer
83B	190	$C_{13}H_{26}$ isomer

(continued)

Table A27 (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
84	190	*n*-tridecane
84A	193	$C_{14}H_{30}$ isomer
84B	197	$C_{14}H_{28}$ isomer
85	198	alkyl butyrate
85A	202	$C_{15}H_{32}$ isomer
85B	205	$C_{15}H_{30}$ isomer
85C	123	$C_{15}H_{30}$ isomer
85D	215	$C_{15}H_{32}$ isomer
85E	216	$C_{15}H_{30}$ isomer
86	217	*n*-pentadecane
87A	229	*n*-hexadecane

[a] See Table 45 for sampling protocol.

APPENDIX B

VAPOR-PHASE HALOGENATED CHEMICALS MEASURED IN AMBIENT AIR

Table B1. VAPOR-PHASE HALOGENATED CHEMICALS - EPA REGION VI

EPA Region	Compound	CASS #	Site	Address	Sampling Time	Calender Day - Year	Conc. (ng/m³)ᵃ
VI	Vinyl chloride	75-01-4	Baton Rouge, LA	Route 190	0940-1140	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	NQ
	Ethyl chloride	75-00-3	Baton Rouge, LA	Route 190	0940-1140	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	NQ
	Vinylidene chloride	75-35-4	Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	6,226
	Methylene chloride	75-09-2	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Baton Rouge, LA	Hw. 61	1210-1410	341-78	
			Baton Rouge, LA	Route 190	0940-1140	342-78	
			Baton Rouge, LA	Route 190	0952-1152	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	NQ
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	W. Port Arthur Rd.	1240-1440	87-79	
			Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Groves, TX	Farm Rd. 366	1210-1410	88-79	
			Beaumont, TX	Spur 380	1125-1325	94-79	
			Beaumont, TX	FM 347	0945-1045	96-79	
			Pasadena, TX	Hw. 225	1000-1130	163-79	
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	
			Deer Park, TX	HW. 225E	1500-1630	165-79	
	Chloroform	67-66-3	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Baton Rouge, LA	Hw. 90 & I-10	0835-0950	45-79	
			Lake Charles, LA	Off I-210	1445-1645	48-79	862
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	W. Port Arthur Rd.	1240-1440	87-79	
			Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Groves, TX	Farm Rd. 366	1210-1410	88-79	
			Beaumont, TX	Spur 380	1125-1325	94-79	
			Beaumont, TX	FM-347	0945-1045	96-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	

(continued)

Table B1 (cont'd.)

EPA Region	Compound	CASS #	Site	Address	Sampling Time	Calender Day - Year	Conc. $(ng/m^3)^a$
	Carbon tetrachloride	56-23-5	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Baton Rouge, LA	Hw. 61	1210-1410	341-78	
			Baton Rouge, LA	Route 190	0940-1140	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Hw. 90 & I-10	0835-0950	45-79	
			Lake Charles, LA	Off I-210	1445-1645	48-79	107
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	W. Port Arthur Rd.	1240-1440	87-79	
			Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Groves, TX	Farm Rd. 366	1210-1410	88-79	749
			Beaumont, TX	Spur 380	1125-1325	97-79	
			Beaumont, TX	FM 347	0945-1045	98-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	6,600
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	1,467
			Deer Park, TX	Hw. 225E	1500-1630	165-79	
	1,2-Dichloroethane	107-06-2	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Hw. 90 & I-10	0835-0950	45-79	
			Lake Charles, LA	Off I-210	1445-1645	48-79	11,516
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	Spur 380	1125-1325	94-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	7,750
			Deer Park, TX	HW. 225E	1500-1630	165-79	700
	1,1,1-Trichloroethane	71-55-6	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Baton Rouge, LA	Hw. 61	1210-1410	341-78	
			Baton Rouge, LA	Route 190	0940-1140	342-78	
			Baton Rouge, LA	Route 190	0952-1152	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Lake Charles, LA	Off I-210	1445-1645	48-79	1,739
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	W. Port Arthur Rd.	1240-1440	87-79	
			Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Groves, TX	Farm Rd. 366	1210-1410	88-79	

(continued)

Table B1 (cont'd.)

EPA Region	Compound	CASS #	Site	Address	Sampling Time	Calender Day - Year	Conc, (ng/m^3)[a]
	1,1,1-Trichloroethane (cont'd.)	71-55-6	Beaumont, TX	Spur 380	1125-1325	94-79	
			Beaumont, TX	FM 347	0945-1045	98-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	560
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	720
			Deer Park, TX	Hw. 225E	1500-1630	165-79	600
	1,1,2-Trichloroethane	79-00-5	Baton Rouge, LA	Route 190	0950-1140	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	3,632
	Trichloroethylene	79-01-6	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Baton Rouge, LA	Route 190	0940-1140	342-78	
			Baton Rouge, LA	Route 190	0952-1152	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Lake Charles, LA	Off I-210	1445-1645	48-79	9,557
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	W. Port Arthur Rd.	1450-1440	87-79	
			Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Groves, TX	RM Rd. 366	1210-1610	88-79	
			Beaumont, TX	Spur 380	1125-1325	94-79	
			Beaumont, TX	FM 347	0945-1045	96-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	3,333
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	3,833
	Tetrachloroethylene	127-18-4	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Baton Rouge, LA	Hw. 61	1210-1410	341-78	
			Baton Rouge, LA	Route 190	0940-1140	342-78	
			Baton Rouge, LA	Route 190	0952-1152	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Lake Charles, LA	Off I-210	1445-1645	48-79	3,504
			Lake Charles, LA	Hw. 90 & I-10	0907-1007	50-79	
			Beaumont, TX	W. Port Arthur Rd.	1240-1440	87-79	
			Baton Rouge, TX	Hw. 61	1150-1350	341-78	
			Groves, TX	FM Rd. 366	1210-1410	88-79	790

(continued)

Table B1 (cont'd.)

EPA Region	Compound	CASS #	Site	Address	Sampling Time	Calender Day - Year	Conc. $(ng/m^3)^a$
	Tetrachloroethylene (cont'd.)	127-18-4	Beaumont, TX	Spur 380	1125-1325	94-79	
			Beaumont, TX	FM 347	0945-1045	96-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	2,269
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	957
			Deer Park, TX	Hw. 225E	1500-1630	165-79	606
	1,1,1,2-Tetrachloroethane		Baton Rouge, LA	Route 190	0940-1140	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	741
	1,1,2,2-Tetrachloroethane		Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	4,947
	Pentachloroethane		Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	273
	Hexachloroethane						
	1,2-Dichloropropane		Groves, TX	Farm Rd. 366	1210-1410	88-79	1,459
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	
	Dichloropropene isomer(s)		Pasadena, TX	Hw. 225E	1000-1130	163-79	
	Trichloropropene isomer(s)		Plaquemine, TX	Route 988	1502-1632	342-78	
	Pentachlorobutadiene		Lake Charles, LA	Off I-210	1445-1645	48-79	713
	1,3-Hexachlorobutadiene	87-68-3	Baton Rouge, LA	Route 190	0940-1140	342-78	
			Plaquemine, LA	Route 988	1502-1632	342-78	
			Lake Charles, LA	Off I-210	1445-1645	48-79	1,312
	Chlorobenzene	108-90-7	Lake Charles, LA	Off I-210	1445-1645	48-79	40
			Beaumont, TX.	W. Port Arthur Rd.	1240-1440	87-79	
			Groves, TX	FM Rd. 366	1210-1410	88-79	1,190
			Pasadena, TX	Hw. 225E	1000-1130	163-79	84
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	
			Deer Park, TX	Hw. 225E	1500-1630	165-79	149

(continued)

Table B1 (cont'd.)

EPA Region	Compound	CASS #	Site	Address	Sampling Time	Calender Day - Year	Conc. (ng/m^3)^a
	Dichlorobenzene isomer(s)	541-73-1	Baton Rouge, LA	Hw. 61	1150-1350	341-78	
		or	Lake Charles, LA	Hw. 90 & I-10	0835-0950	45-79	
		95-50-1	Lake Charles, LA	Off I-210	1445-1645	48-79	25
			Beaumont, TX	W. Port Arthur Rd.	1240-1440	87-79	
			Baton Rouge, LA	Hw. 61	1150-1350	341-78	
			Groves, TX	FM 366	1210-1410	88-79	
			Beaumont, TX	Spur 380	1125-1325	94-79	
			Beaumont, TX	FM 347	0945-1045	96-79	
			Pasadena, TX	Hw. 225E	1000-1130	163-79	T
			Pasadena, TX	Off Rickey St.	1430-1600	164-79	
	Trichlorobenzene isomer(s)	12002-48-1	Baton Rouge, LA	Hw. 61	1150-1350	341-78	8
	Chlorotoluene isomer(s)		Baton Rouge, LA	Hw. 61	1150-1350	341-78	
	Benzyl chloride (tent.)		Baton Rouge, LA	Hw. 61	1150-1350	341-78	
	1,2-Dibromoethane	106-93-4	Beaumont, TX	Spur 380	1125-1325	94-79	
	Pentachlorobromoethane (tent.)		Lake Charles, LA	Off I-210	1445-1645	48-79	347